Generative Models

Foundations | Tricks | Algorithms

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Principles to Products

Applications: Assistive Technology | Advancing Science | Climate and Energy | Healthcare | Fairness and Safety | Autonomous systems

Reasoning: Planning | Explanation | Rapid Learning | World Simulation | Objects and Relations

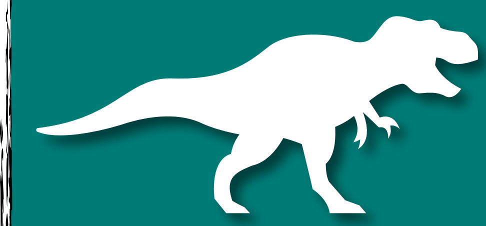
Information: Uncertainty | Information Gain | Causality | Prediction

Principles: Probability Theory | Bayesian Analysis | Hypothesis Testing | Estimation Theory | Asymptotics

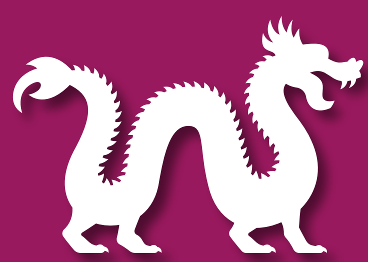
Generative Models

Part I: Foundations

Learning Objectives



1. Language to think about the Philosophy of Machine Learning



2. Understand the Model-Inference-Algorithm paradigm

Probability

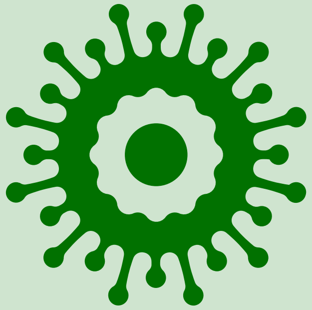
Some Definitions for probability

Statistical Probability

Frequency ratio of items

Logical Probability

Degree of confirmation of a hypothesis based on logical analysis



Probability as Propensity

Probability used for predictions

Subjective Probability

Probability as a degree of belief

Probability is sufficient for the task of reasoning under uncertainty

Probability

Probability as a Degree of Belief

Probability is a measure of the belief in a proposition **given** evidence.
A description of a state of knowledge.

No such thing as **the probability** of an event, since the value depends on the evidence used.

Inherently subjective in that it depends on the believer's information

Different observers with different information will have different beliefs.

Probabilistic Quantities

Probability $p(\mathbf{x}) \qquad p^*(\mathbf{x}) \qquad q(\mathbf{x})$

Conditions $p(\mathbf{x}) \geq 0 \qquad \int p(\mathbf{x}) d\mathbf{x} = 1$

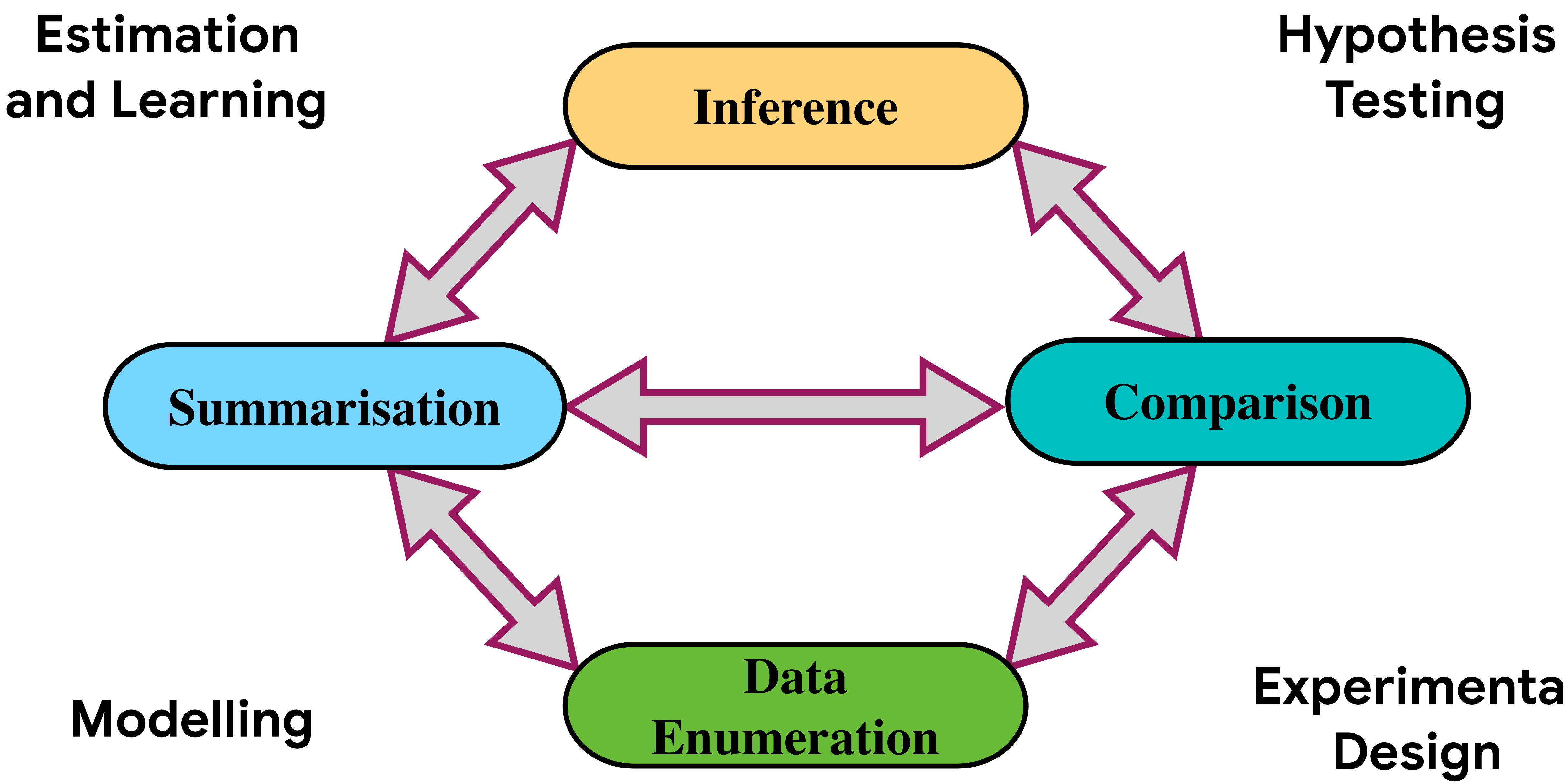
Bayes Rule $$p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{p(\mathbf{x})}$$

Parameterisation $$p_\theta(\mathbf{x}|\mathbf{z}) \equiv p(\mathbf{x}|\mathbf{z};\boldsymbol{\theta})$$

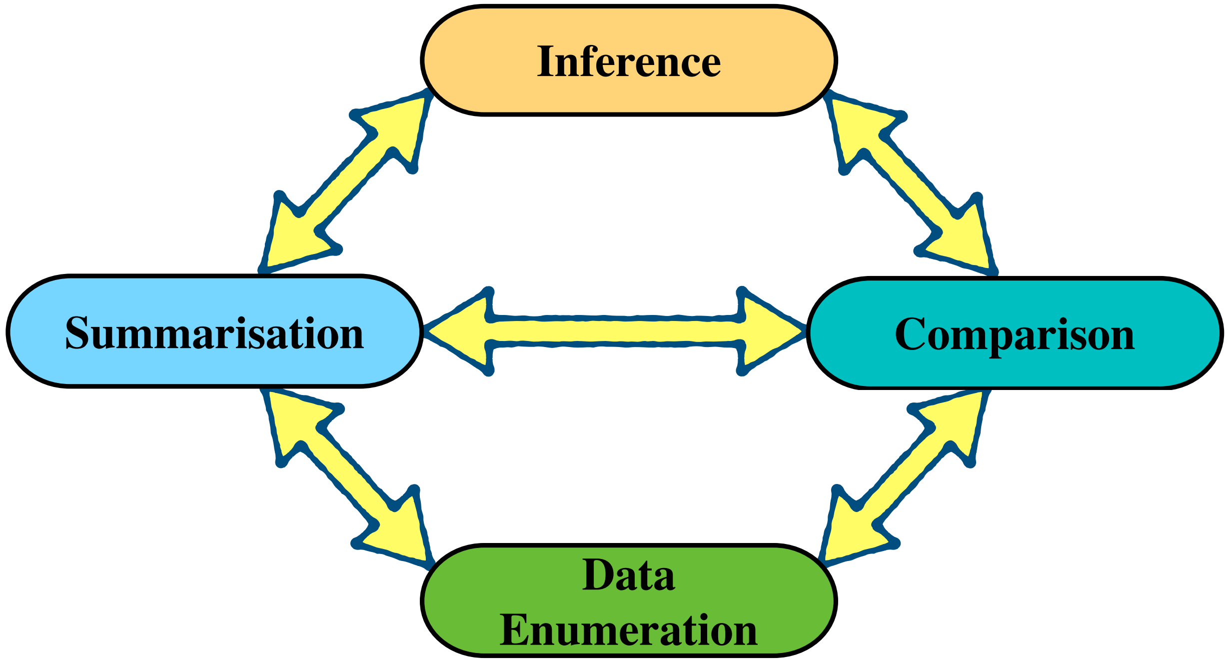
Expectation $$\mathbb{E}_{p_\theta(\mathbf{x}|\mathbf{z})}[f(\mathbf{x};\phi)] = \int p_\theta(\mathbf{x}|\mathbf{z}) f(\mathbf{x};\phi) d\mathbf{x}$$

Gradient $$\nabla_\phi f(\mathbf{x};\phi) = \frac{\partial f(\mathbf{x};\phi)}{\partial \phi}$$

Statistical Operations



Centrality of Inference



Artificial General Intelligence will be the refined instantiation of these statistical operations.

The core questions of AGI will be those of probabilistic inference

Foundations

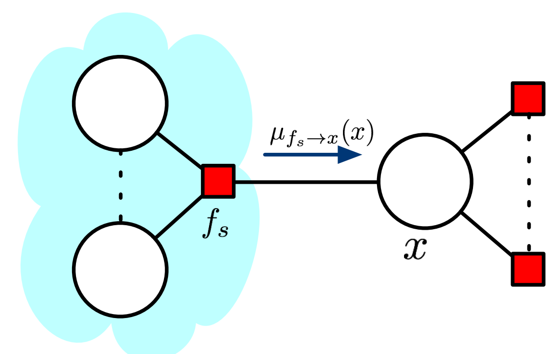
How will you approach your ML research and practice?

In general:
Human-centred,
interdisciplinary approach

- Sociological
- Psychological
- Componential
- Physiological

Sun's Phenomenological Levels

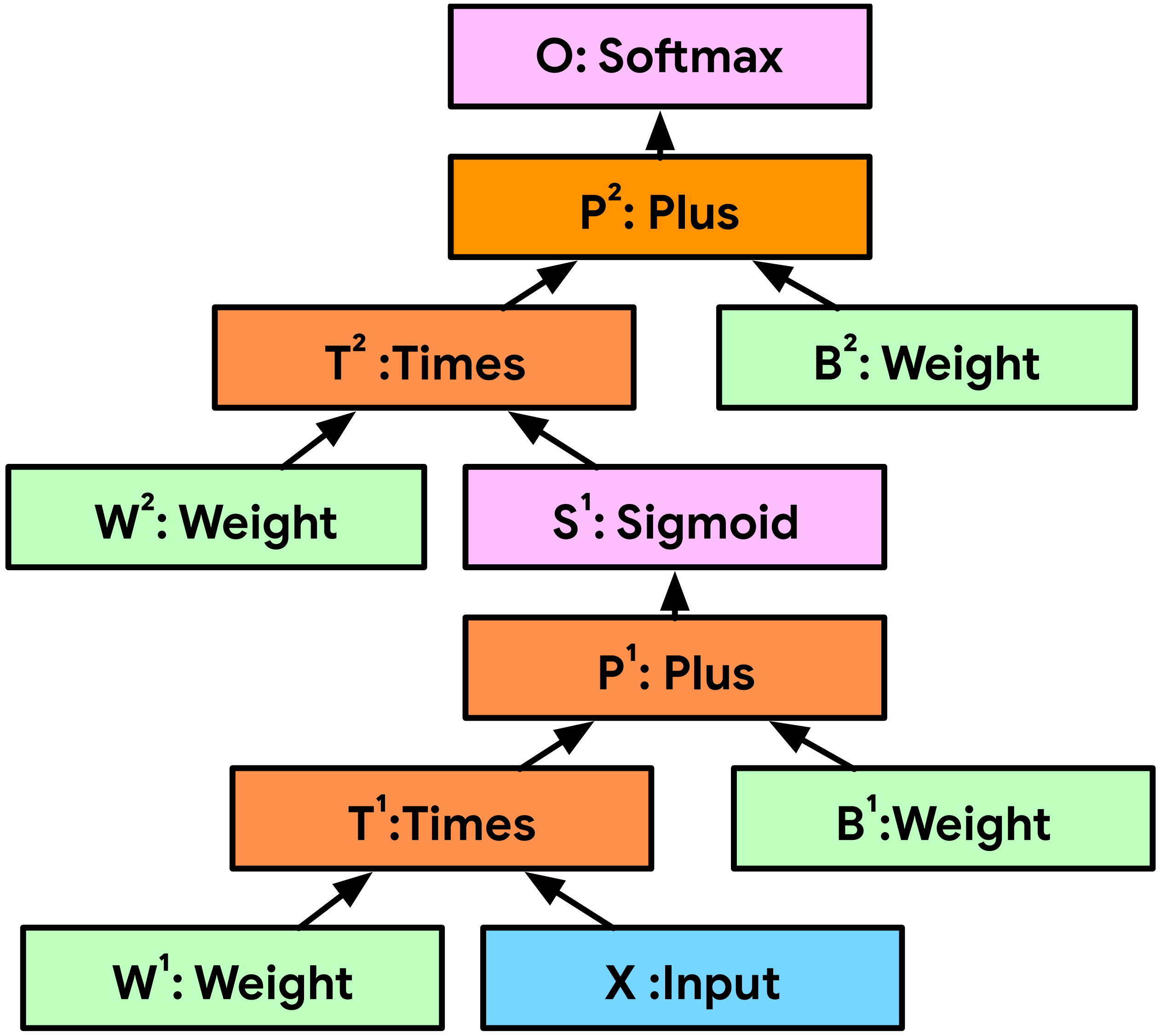
For the ML Core:
Probabilistic and pragmatic in approach



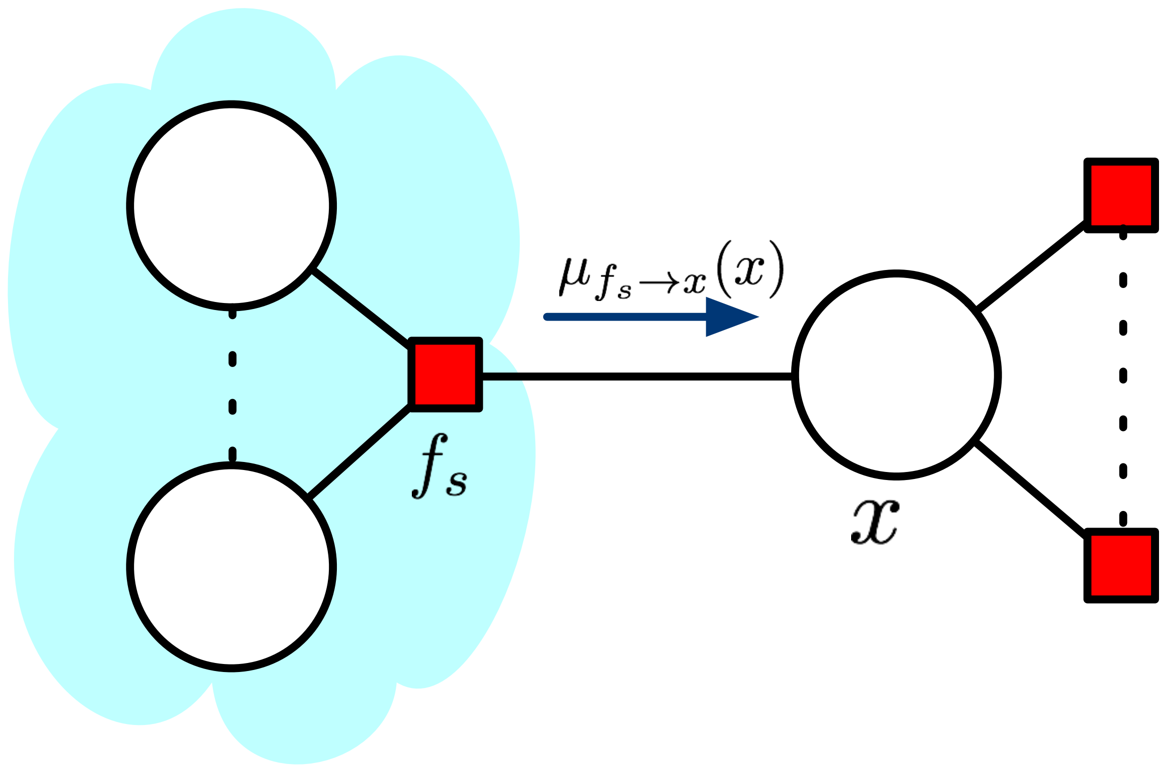
Architecture-Loss

Model-Inference-Algorithm

Architecture-Loss

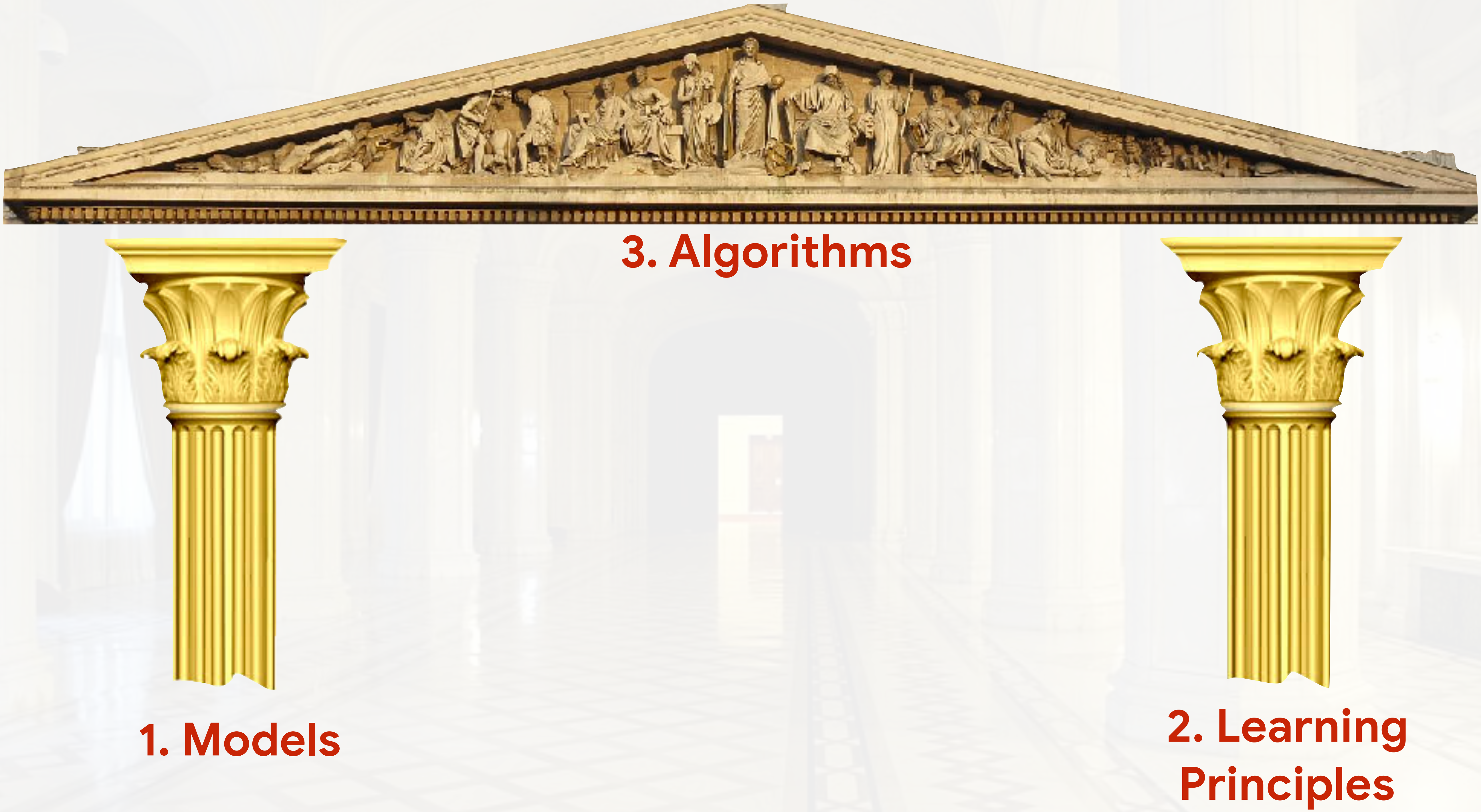


1. Computational Graphs



2. Error propagation

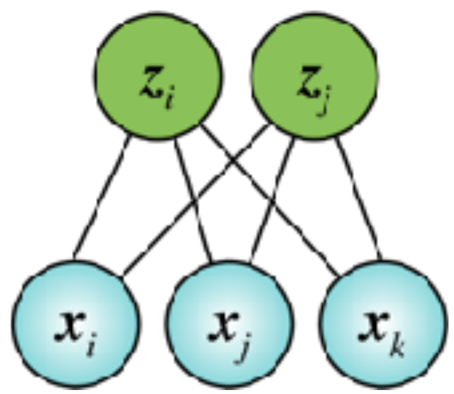
Model-Inference-Algorithm

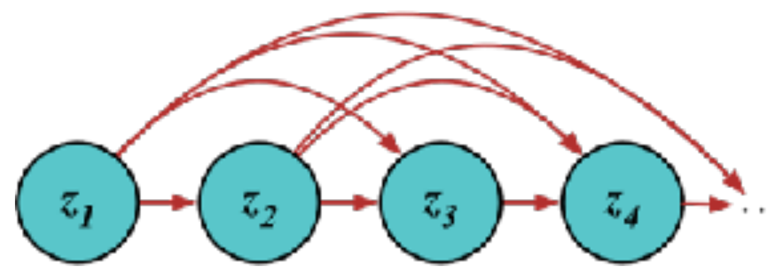


Models

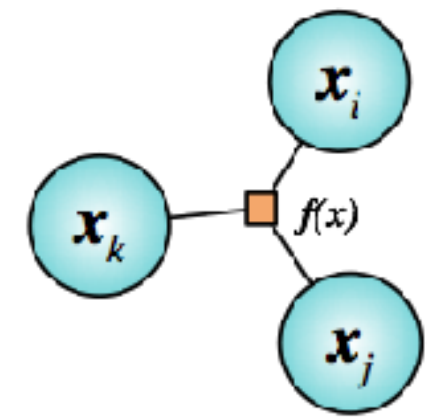
Models

Directed and Undirected

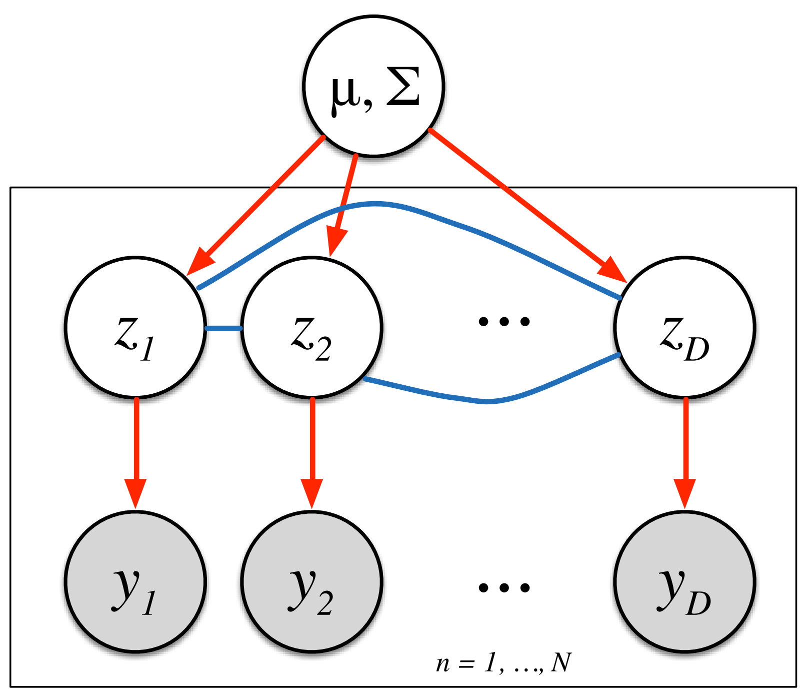




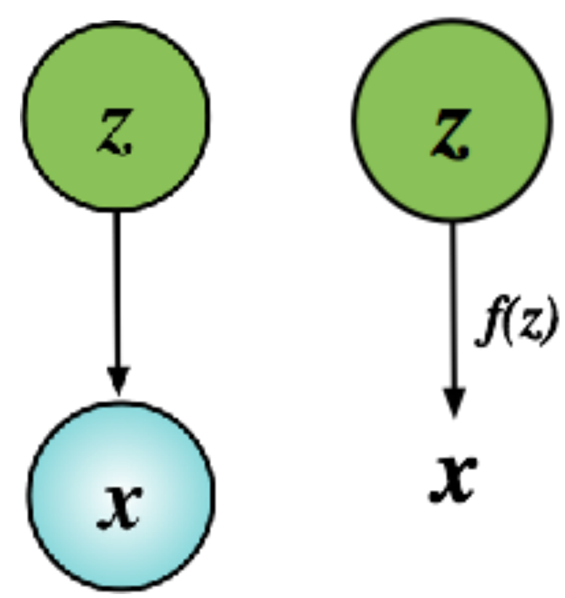
Fully-observed



Parametric, Non-parametric And semi-parametric



Latent Variable



Learning Principles

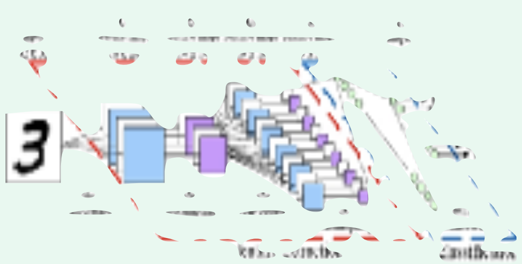
- **Statistical Inference**
  - **Direct**
    - Laplace approximation
    - Maximum Likelihood
    - Maximum a posteriori
    - Variational Inference
    - Cavity Methods
    - Integr. Nested Laplace Approx
    - Expectation Maximisation
    - Markov chain Monte Carlo
    - Noise Contrastive
    - Sequential Monte Carlo
  - **Indirect**
    - Two Sample Comparison
    - Method of Moments
    - Approx Bayesian Computation
    - Transportation methods
    - Max Mean Discrepency

Learning Principles

Algorithms

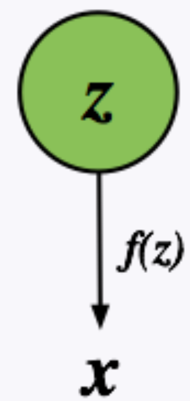
A given model and learning principle can be implemented in many ways.

Convolutional neural network + penalised maximum likelihood



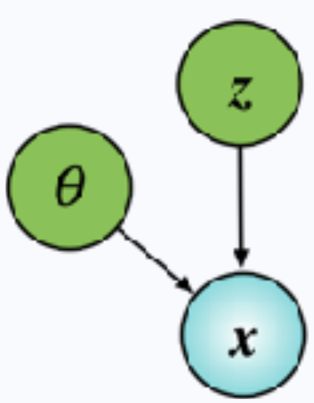
- Optimisation methods (SGD, Adagrad)
- Regularisation (L1, L2, batchnorm, dropout)

Implicit Generative Model + Two-sample testing



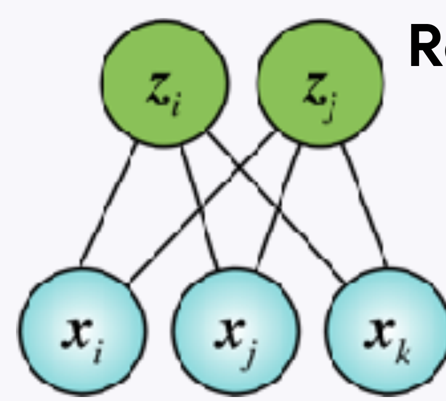
- Unsupervised-as-supervised learning
- Approximate Bayesian Computation (ABC)
- Generative adversarial network (GAN)

Latent variable model + variational inference



- VEM algorithm
- Expectation propagation
- Approximate message passing
- Variational auto-encoders (VAE)

Restricted Boltzmann Machine + maximum likelihood

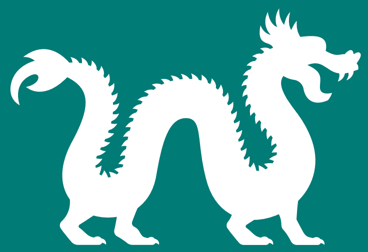


- Contrastive Divergence
- Persistent CD
- Parallel Tempering
- Natural gradients

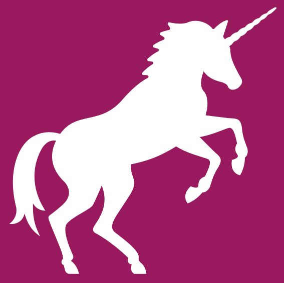
Generative Models

Part II: Tricks

Learning Objectives



1. Develop tools to manipulate distributions by studying 4 probability questions.



2. Build connections between concepts in machine learning and those in other computational sciences.

Inferential Questions

Probabilistic dexterity is needed to solve the fundamental problems of machine learning and artificial intelligence.

Evidence Estimation

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) dz$$

Moment Computation

$$\mathbb{E}[f(\mathbf{z})|\mathbf{x}] = \int f(\mathbf{z}) p(\mathbf{z}|\mathbf{x}) dz$$

Parameter Estimation

$$p(\boldsymbol{\theta}|\mathbf{x}_{0:N})$$

Prediction

$$p(\mathbf{x}_{t+1}|\mathbf{x}_{0:t})$$

Planning

$$\mathcal{J} = \mathbb{E}_p \left[\int_0^\infty C(\mathbf{x}_t) dt | \mathbf{x}_0, \mathbf{u} \right]$$

Hypothesis Testing

$$\mathcal{B} = \log p(\mathbf{x}|H_1) - \log p(\mathbf{x}|H_2)$$

Experimental Design

$$\mathcal{IG} = D[p(\mathbf{x}_{t:T}|u) \| p(\mathbf{x}_{0:t})]$$

Identity Trick

Transform an expectation w.r.t. distribution *p*,
into an expectation w.r.t. distribution *q*.

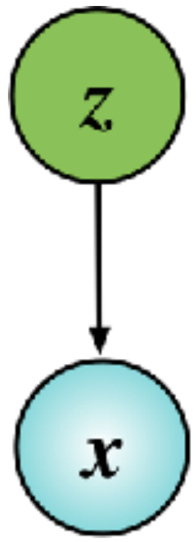
$$\int p(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} = \mathbb{E}_{p(\mathbf{x})}[f(\mathbf{x})]$$

$$\updownarrow$$

$$\mathbb{E}_{q(\mathbf{x})}[g(\mathbf{x}; f)] = \int q(\mathbf{x}) g(\mathbf{x}, f) d\mathbf{x}$$

Do this by introducing a **probabilistic one** $\frac{p(\mathbf{x})}{p(\mathbf{x})}$

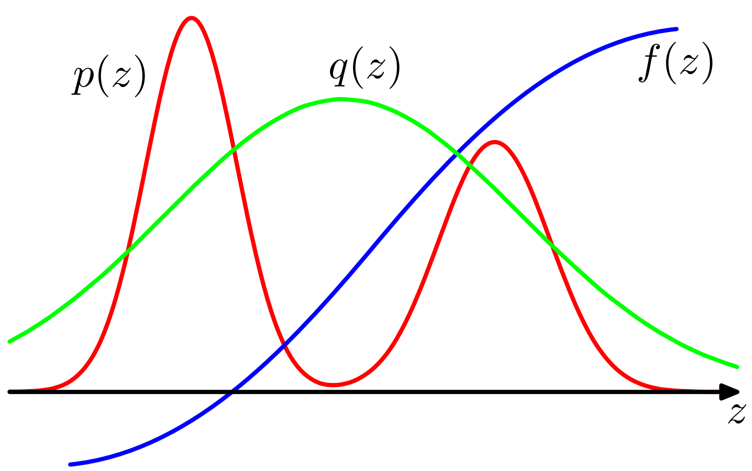
Identity Trick



Integral problem $$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$$

Probabilistic one $$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})\boxed{\frac{q(\mathbf{z})}{q(\mathbf{z})}}d\mathbf{z}$$

Re-group/re-weight $$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})\boxed{\frac{p(\mathbf{z})}{q(\mathbf{z})}}q(\mathbf{z})d\mathbf{z}$$



Conditions

- *q(z)*>0, when p(x|*z)p(z)* $\neq 0$.
- *q(z) is known/easy to handle.*

$$p(\mathbf{x}) = \mathbb{E}_{q(\mathbf{z})}\left[p(\mathbf{x}|\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})}\right]$$

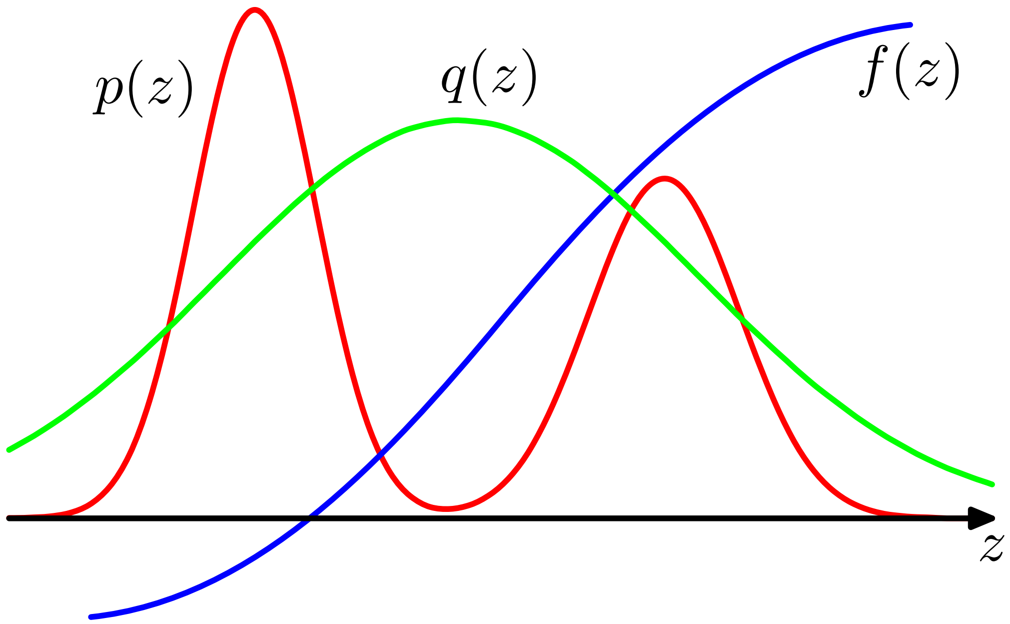
Importance Sampling

$$p(\mathbf{x}) = \mathbb{E}_{q(\mathbf{z})}\left[p(\mathbf{x}|\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})}\right]$$

Monte Carlo Estimator

$$p(\mathbf{x}) = \frac{1}{S}\sum_s w^{(s)} p(\mathbf{x}|\mathbf{z}^{(s)})$$

$$w^{(s)} = \frac{p(z)}{q(z)} \quad z^{(s)} \sim q(z)$$

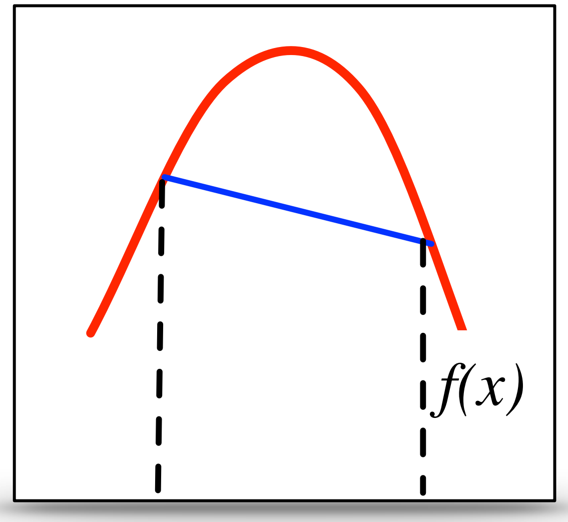


Identity Trick Elsewhere

- Manipulate stochastic gradients
- Derive probability bounds
- RL for policy corrections

Bounding Tricks

An important result from convex analysis lets us move expectations through a function:



For concave functions $f(.)$

$$f(\mathbb{E}[x]) \geq \mathbb{E}[f(x)]$$

Logarithms are strictly *concave* allowing us to use Jensen's inequality.

$$\log \int p(x) g(x) dx \geq \int p(x) \log g(x) dx$$

Bounding Trick Elsewhere

Optimisation; Variational Inference; Rao-Blackwell Theorem;

Other Bounding Tricks

- Fenchel duality
- Holder's inequality
- Monge-Kantorovich Inequality

Evidence Bounds

Integral problem

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$$

Proposal

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})\frac{q(\mathbf{z})}{q(\mathbf{z})}d\mathbf{z}$$

Importance Weight

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})}q(\mathbf{z})d\mathbf{z}$$

Jensen's inequality

$$\log \int p(x)g(x)dx \geq \int p(x) \log g(x)dx$$

$$\log p(\mathbf{x}) \geq \int q(\mathbf{z}) \log \left(p(\mathbf{x}|\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})} \right) d\mathbf{z}$$

$$= \int q(\mathbf{z}) \log p(\mathbf{x}|\mathbf{z}) - \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z})}$$

Lower bound

$$\mathbb{E}_{q(\mathbf{z})}[\log p(\mathbf{x}|\mathbf{z})] - KL[q(\mathbf{z})\|p(\mathbf{z})]$$

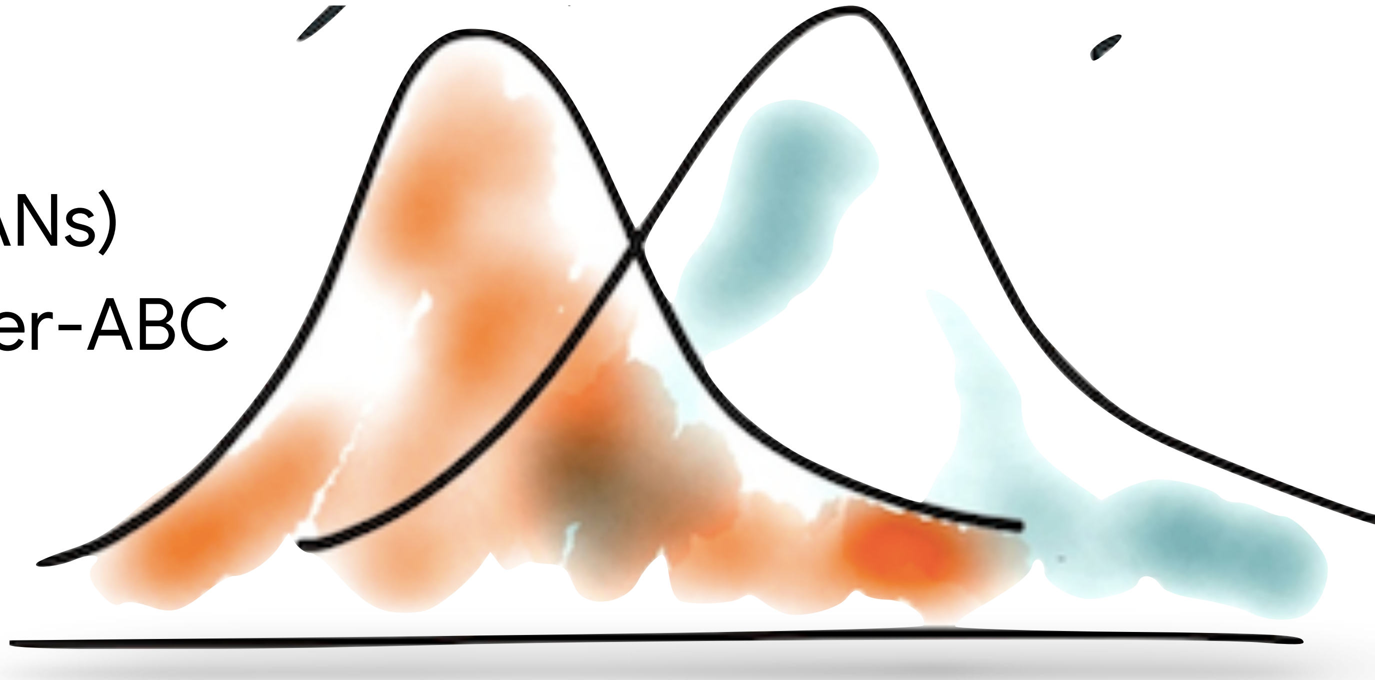
Density Ratio Trick

The ratio of two densities can be computed using a classifier of using samples drawn from the two distributions.

$$\frac{p^*(\mathbf{x})}{q(\mathbf{x})} = \frac{p(y=1|\mathbf{x})}{p(y=-1|\mathbf{x})}$$

Density Ratio Trick Elsewhere

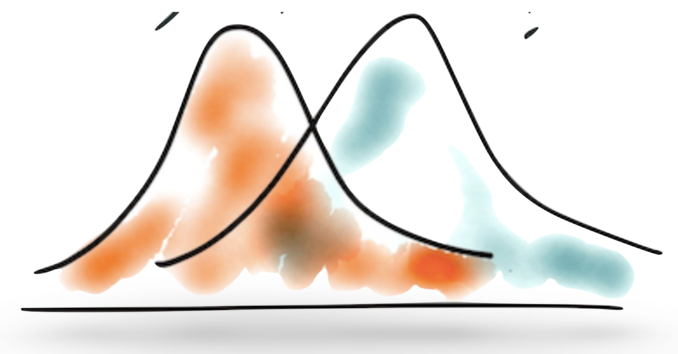
- Generative Adversarial Networks (GANs)
- Noise contrastive estimation, Classifier-ABC
- Two-sample testing
- Covariate-shift, calibration



Density Ratio Estimation

Assign labels $\{y_1, \ldots, y_N\} = \{+1, \ldots, +1, -1, \ldots, -1\}$

Equivalence $p^*(\mathbf{x}) = p(\mathbf{x}|y=1) \qquad q(\mathbf{x}) = p(\mathbf{x}|y=-1)$



Density Ratio $\dfrac{p^*(\mathbf{x})}{q(\mathbf{x})}$ **Bayes' Rule** $p(\mathbf{x}|y) = \dfrac{p(y|\mathbf{x})p(\mathbf{x})}{p(y)}$

Conditional

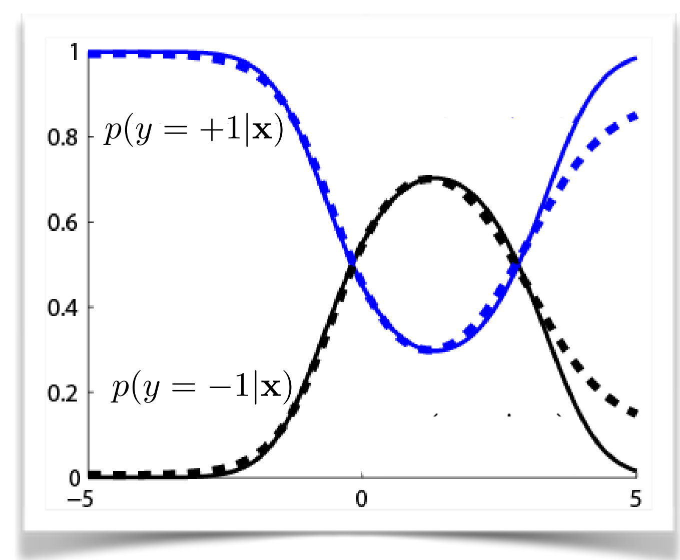
$$\frac{p^*(\mathbf{x})}{q(\mathbf{x})} = \frac{p(\mathbf{x}|y=1)}{p(\mathbf{x}|y=-1)}$$

Bayes' Subst.

$$= \frac{p(y=+1|\mathbf{x})p(\mathbf{x})}{p(y=+1)} \Big/ \frac{p(y=-1|\mathbf{x})p(\mathbf{x})}{p(y=-1)}$$

Class probability

$$\frac{p^*(\mathbf{x})}{q(\mathbf{x})} = \boxed{\frac{p(y=1|\mathbf{x})}{p(y=-1|\mathbf{x})}}$$



Computing a density ratio is equivalent to class probability estimation.

Stochastic Optimisation

Common gradient problem

$$\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z})}[f_\theta(\mathbf{z})] = \nabla \int \boxed{q_\phi(\mathbf{z})}\boxed{f_\theta(\mathbf{z})} d\mathbf{z}$$

- Don’t know this expectation in general.
- Gradient is of the parameters of the distribution w.r.t. which the expectation is taken.

1. **Pathwise estimator**: Differentiate the function **f(z)**
2. **Score-function estimator**: Differentiate the density **q(z|x)**

Typical problem areas

- Sensitivity analysis
- Generative models and inference
- Reinforcement learning and control
- Operations research and inventory control
- Monte Carlo simulation
- Finance and asset pricing

Log-derivative Trick

Score function is the derivative of a log-likelihood function.

$$\nabla_\phi \log q_\phi(\mathbf{z}) = \frac{\nabla_\phi q_\phi(\mathbf{z})}{q_\phi(\mathbf{z})}$$

Several useful properties

Expected score $\mathbb{E}_{q(z)}\left[\nabla_\phi \log q_\phi(\mathbf{z})\right] = 0$ **↞Show this**

$$\mathbb{E}_{q(z)}[\nabla_\phi \log q_\phi(\mathbf{z})] = \int q(z) \frac{\nabla_\phi q_\phi(\mathbf{z})}{q_\phi(\mathbf{z})} = \nabla \int q_\phi(\mathbf{z}) = \nabla 1 = 0$$

Fisher Information $\mathbb{V}[\nabla_\theta \log p(\mathbf{x};\theta)] = \mathcal{I}(\theta) = \mathbb{E}_{p(x;\theta)}[\nabla_\theta \log p(\mathbf{x};\theta) \nabla_\theta \log p(\mathbf{x};\theta)^\top]$

Score-function Estimator

$$\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z})}[f_\theta(\mathbf{z})] = \nabla \int \boxed{q_\phi(\mathbf{z})} f_\theta(\mathbf{z}) d\mathbf{z}$$

Leibnitz integral rule

$$= \int \frac{q_\phi(\mathbf{z})}{q_\phi(\mathbf{z})} \nabla_\phi q_\phi(\mathbf{z}) f(\mathbf{z}) d\mathbf{z}$$

Identity

$$= \int q_\phi(\mathbf{z}) \nabla_\phi \log q_\phi(\mathbf{z}) f(\mathbf{z}) d\mathbf{z}$$

Log-deriv

$$= \mathbb{E}_{q_\phi(\mathbf{z})} \left[f(\mathbf{z}) \nabla_\phi \log q_\phi(\mathbf{z}) \right]$$

Gradient

$$\boxed{\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z})}[f_\theta(\mathbf{z})] = \mathbb{E}_{q_\phi(\mathbf{z})} \left[(f(\mathbf{z}) - c) \nabla_\phi \log q_\phi(\mathbf{z}) \right]}$$

Control Variate

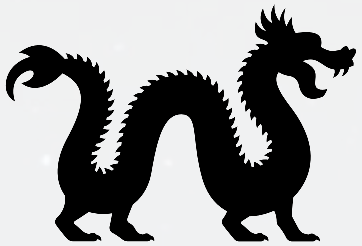
Other names

- Likelihood ratio method
- REINFORCE and policy gradients
- Automated & Black-box inference

When to use

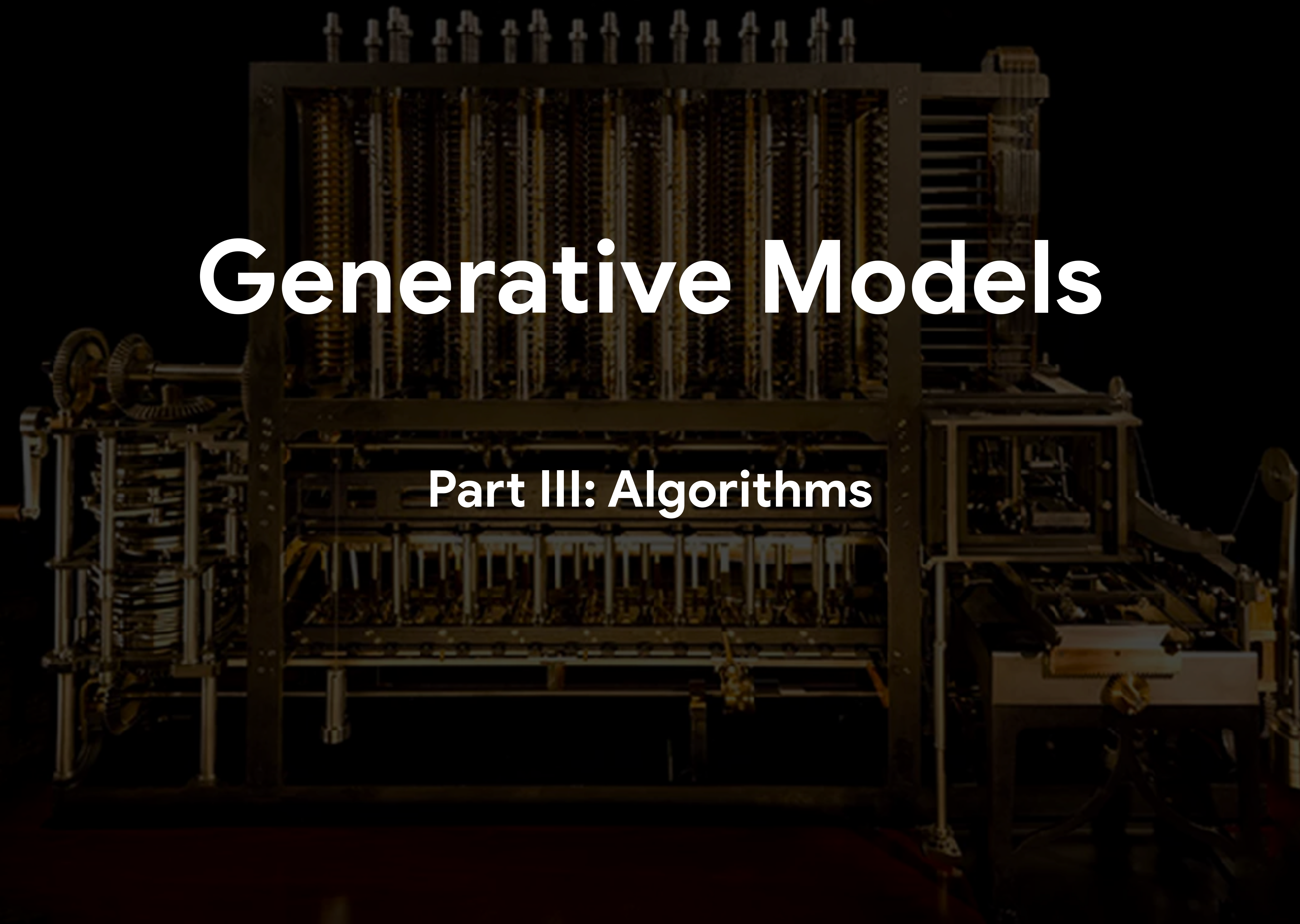
- Function is not differentiable, not analytical.
- Distribution *q* is easy to sample from.
- Density *q* is known and differentiable.

Many More Tricks



Strengthen your probabilistic dexterity.

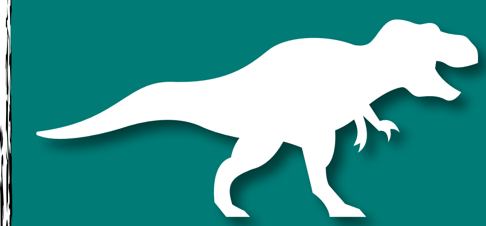
Identity	$\frac{p(\mathbf{x})}{p(\mathbf{x})}$
Hutchinson's	$\mathbb{E}[\mathbf{z}\mathbf{z}^\top] = \mathbf{I}$
Flows	$p(\mathbf{y}) = p(\mathbf{x}) \left\| \frac{dg}{d\mathbf{x}} \right\|^{-1}$
Log-derivative	$\nabla_\phi \log q_\phi(\mathbf{z}) = \frac{\nabla_\phi q_\phi(\mathbf{z})}{q_\phi(\mathbf{z})}$
Reparameterisation	$\mathbf{z} = g(\epsilon, \phi) \quad \epsilon \sim p(\epsilon)$
Density Ratio	$\frac{p^*(\mathbf{x})}{q(\mathbf{x})} = \frac{p(y=1\|\mathbf{x})}{p(y=-1\|\mathbf{x})}$



Generative Models

Part III: Algorithms

Learning Objectives



1. Have knowledge of different types of probabilistic models for unsupervised learning.

2. Build awareness of the breadth of applications of generative models.

Beyond Classification

Move beyond associating inputs to outputs

Understand and simulate how the world evolves

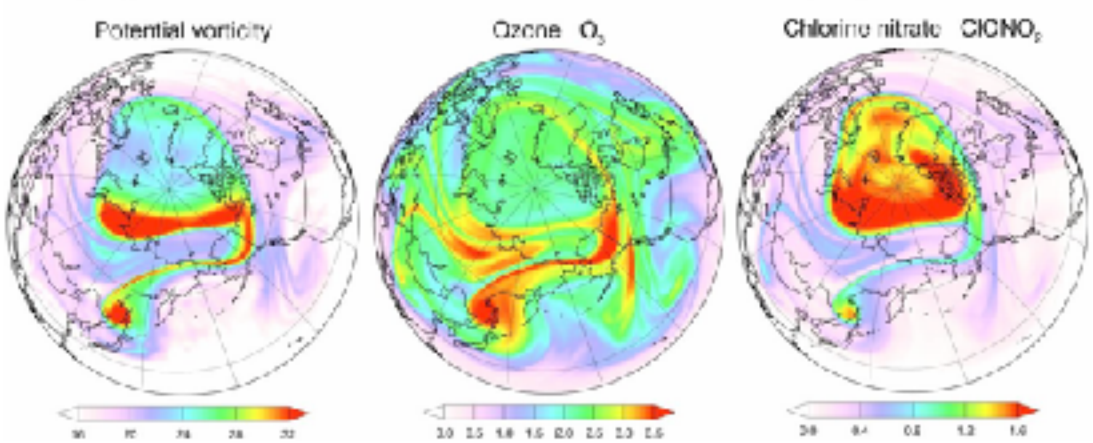
Recognise objects in the world and their factors of variation

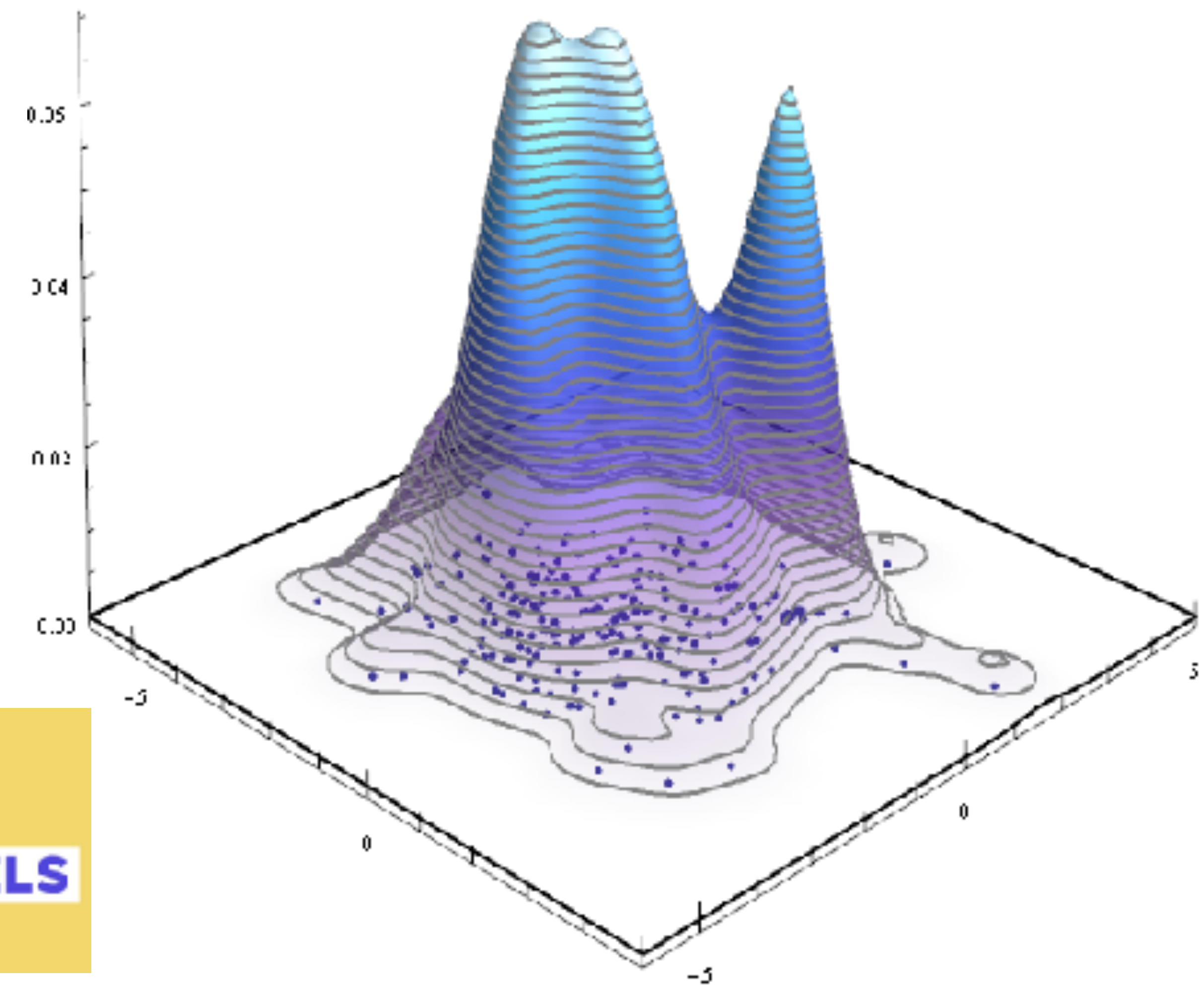
Detect surprising events in the world

Establish concepts as useful for reasoning and decision making

Anticipate and generate rich plans for the future

Generative Models





NO LABELS

A model that allows us to learn a simulator of data

Models that allow for (conditional) density estimation

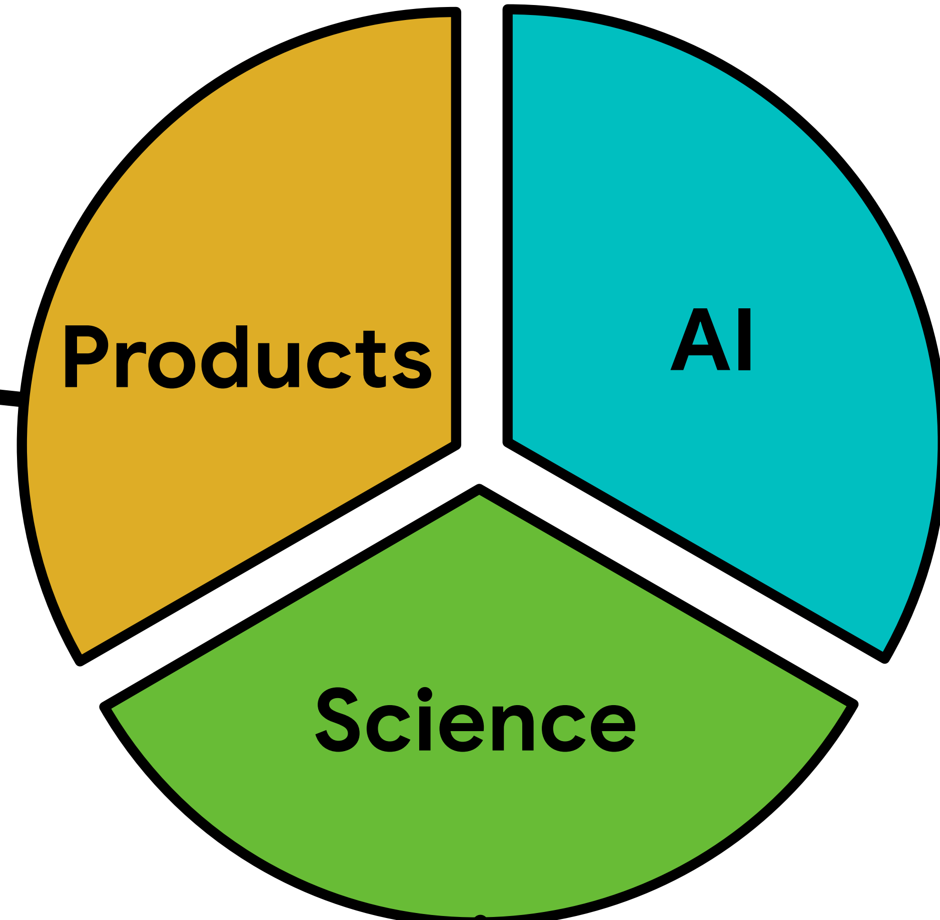
Approaches for unsupervised learning of data

Characteristics are:

- **Probabilistic** models of data that allow for uncertainty to be captured.
- **High-dimensional** data.
- **Data distribution** is targeted.

Applications

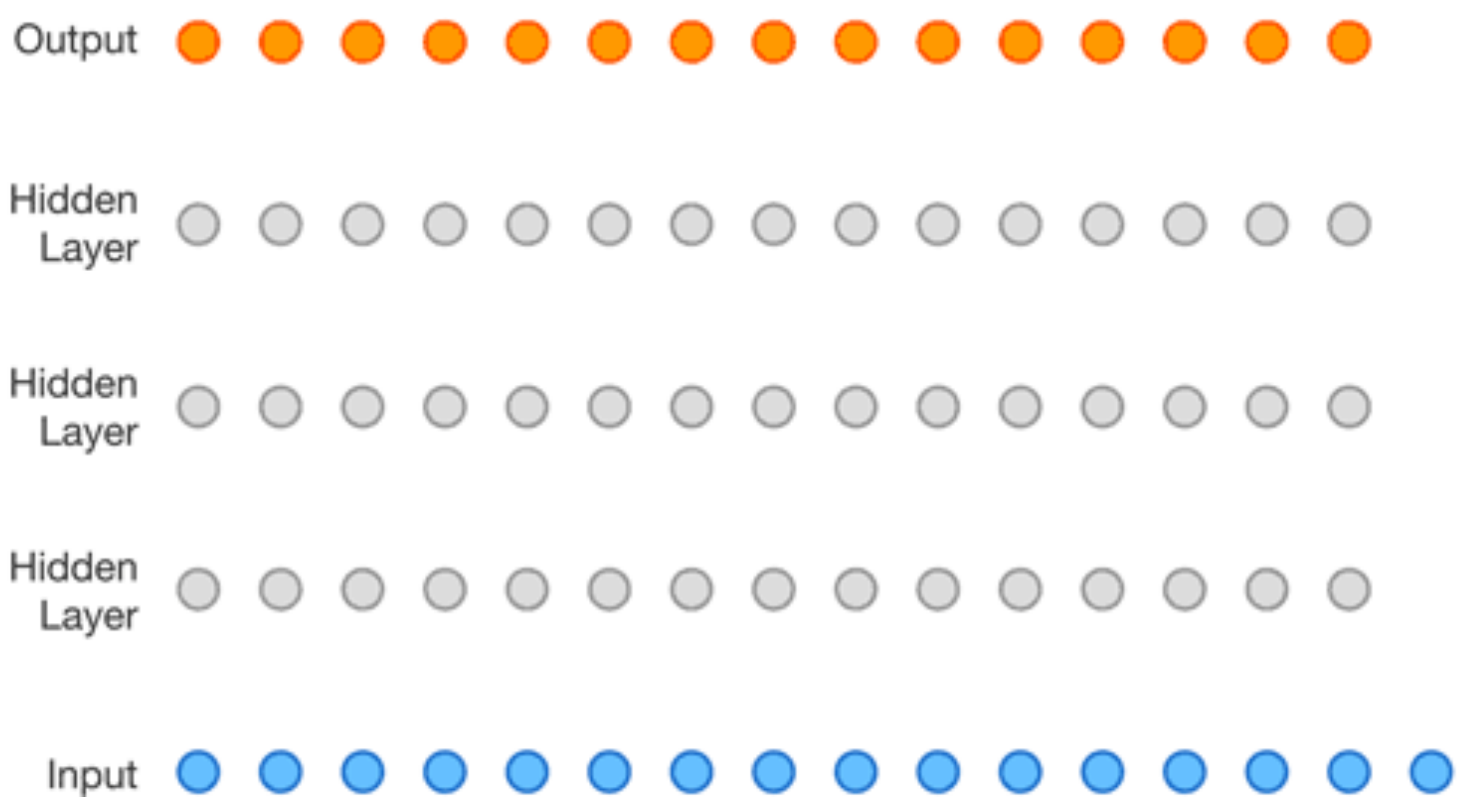
Super-resolution,
Compression,
Text-to-speech

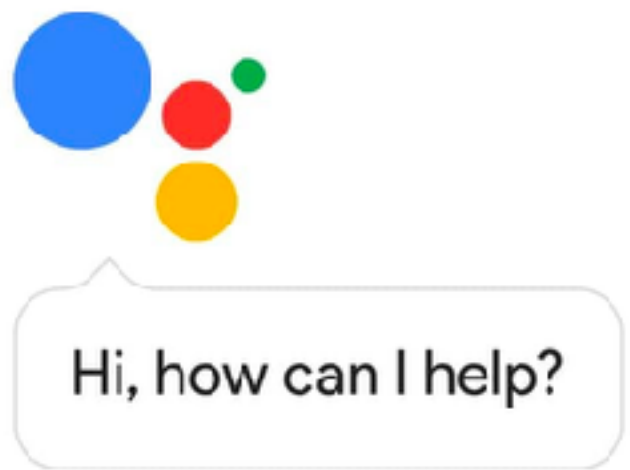


Planning,
Exploration
Intrinsic motivation
Model-based RL

Proteomics,
Drug Discovery,
Astronomy,
High-energy physics

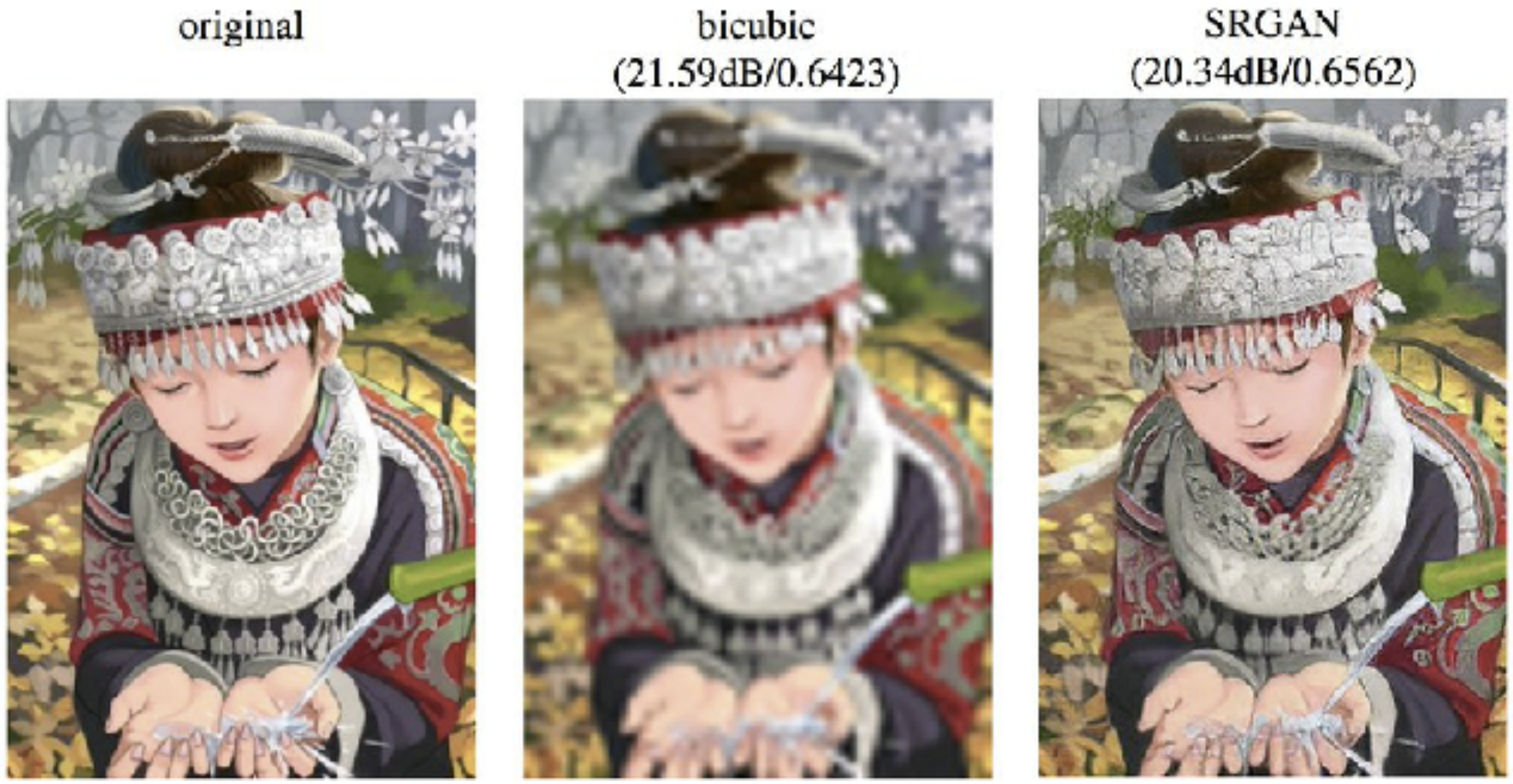
Assistive Technologies

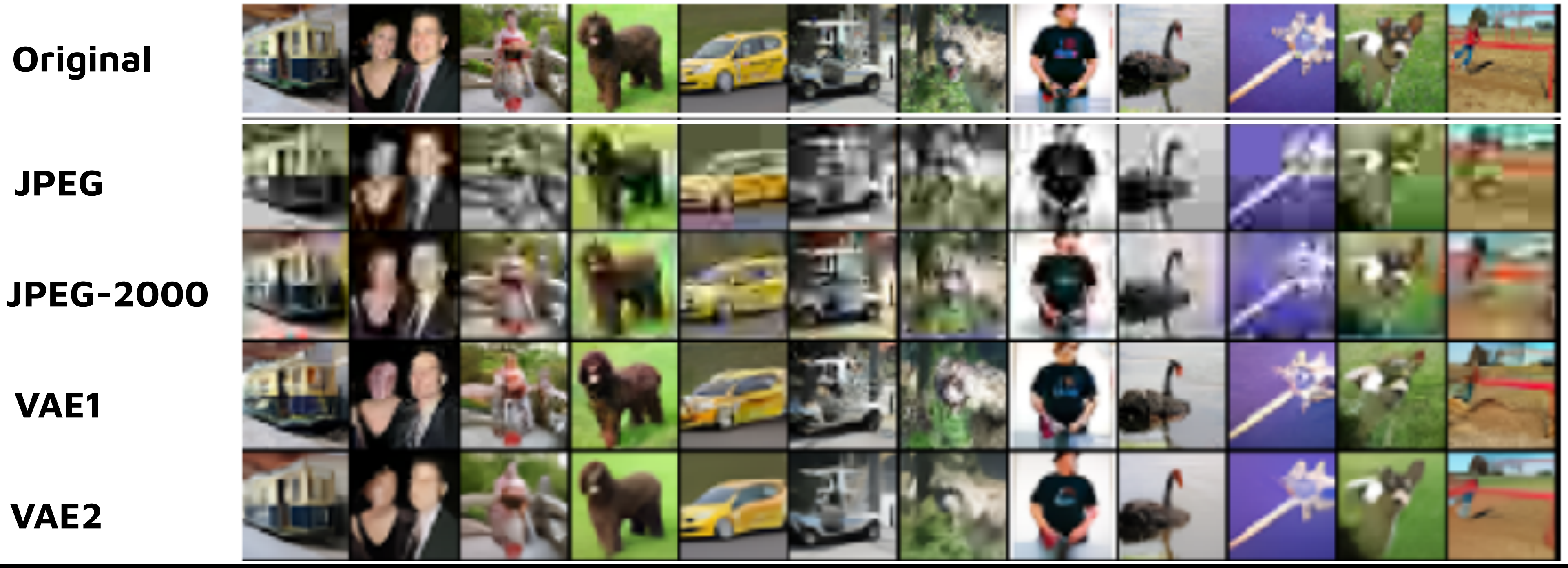




Fully-observed conditional generative model

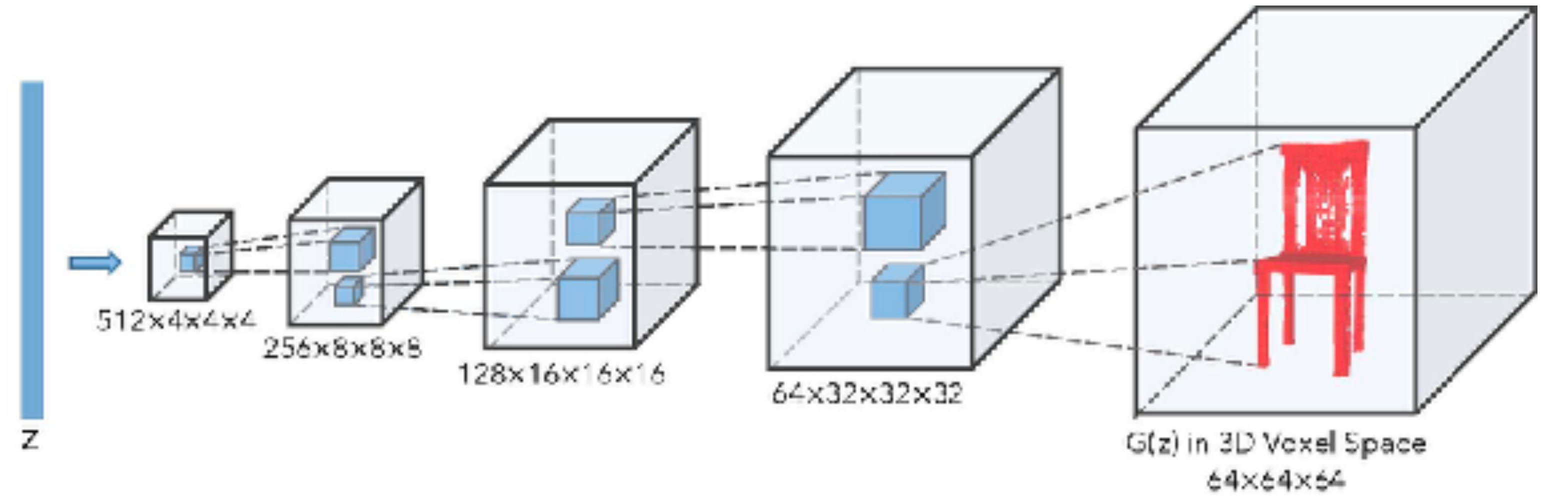
Compression-Communication

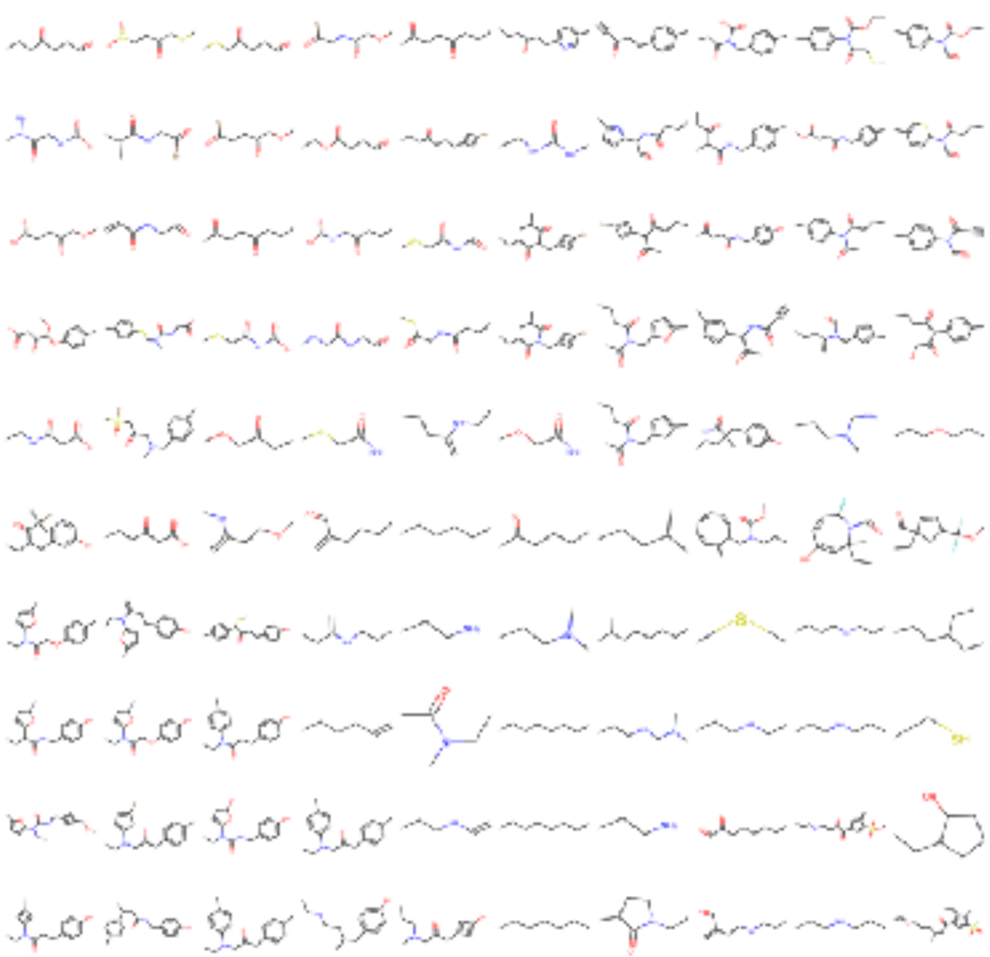


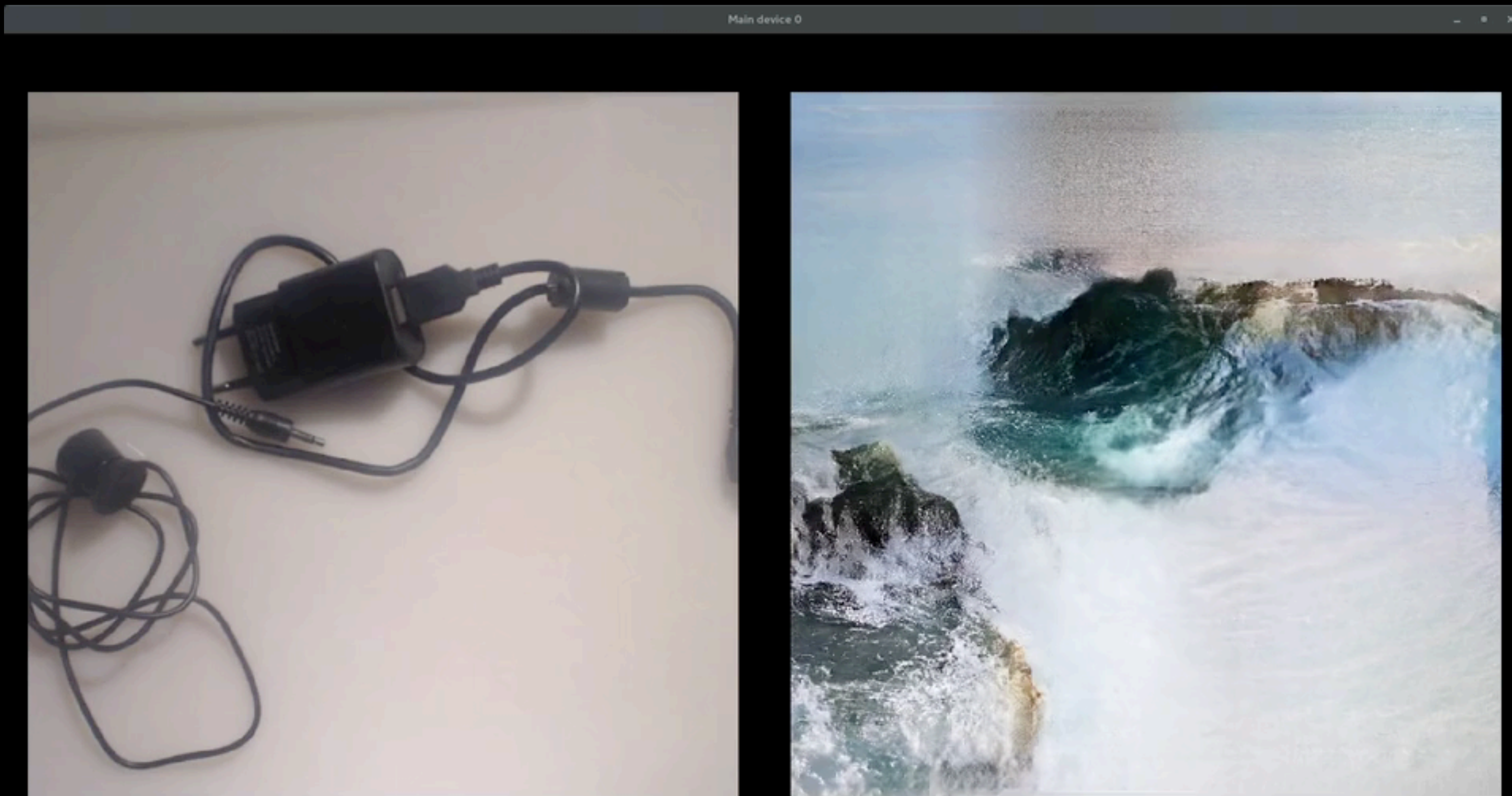


Compression rate: 0.2bits/dimension

Generative Design

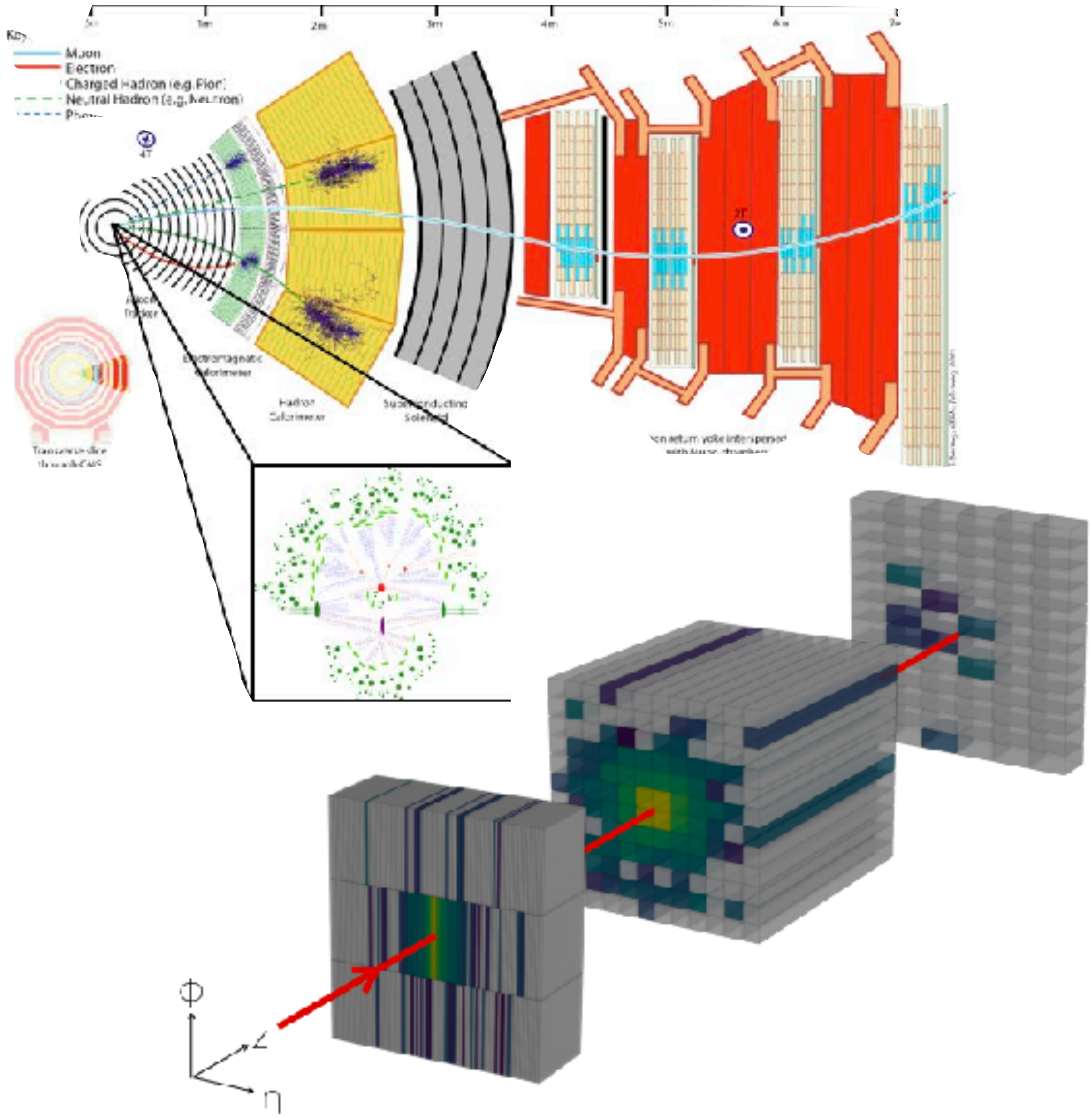


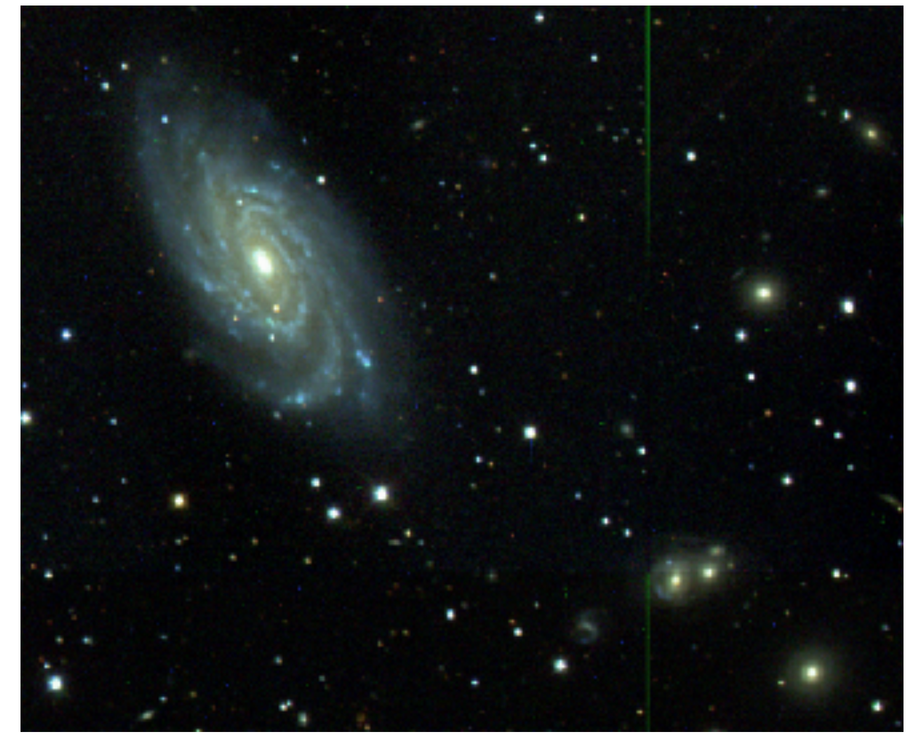


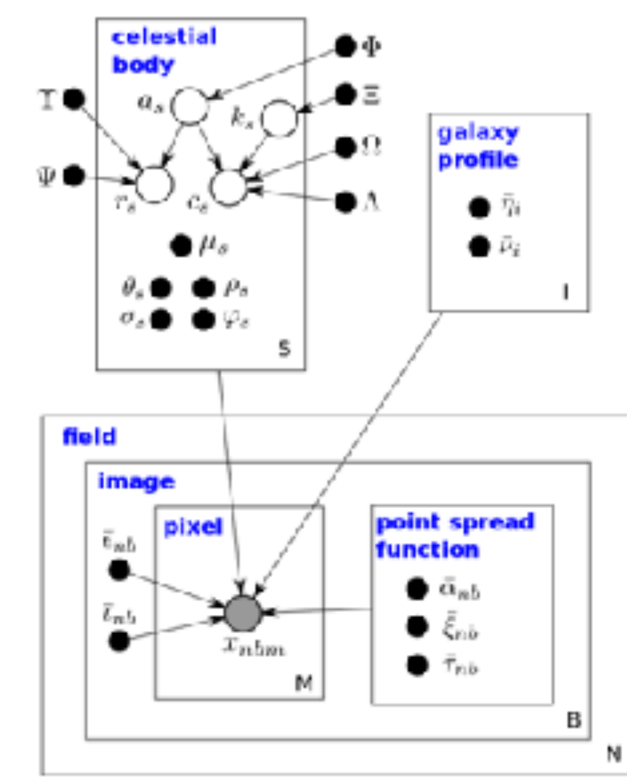


Video from work of Memo Aktem

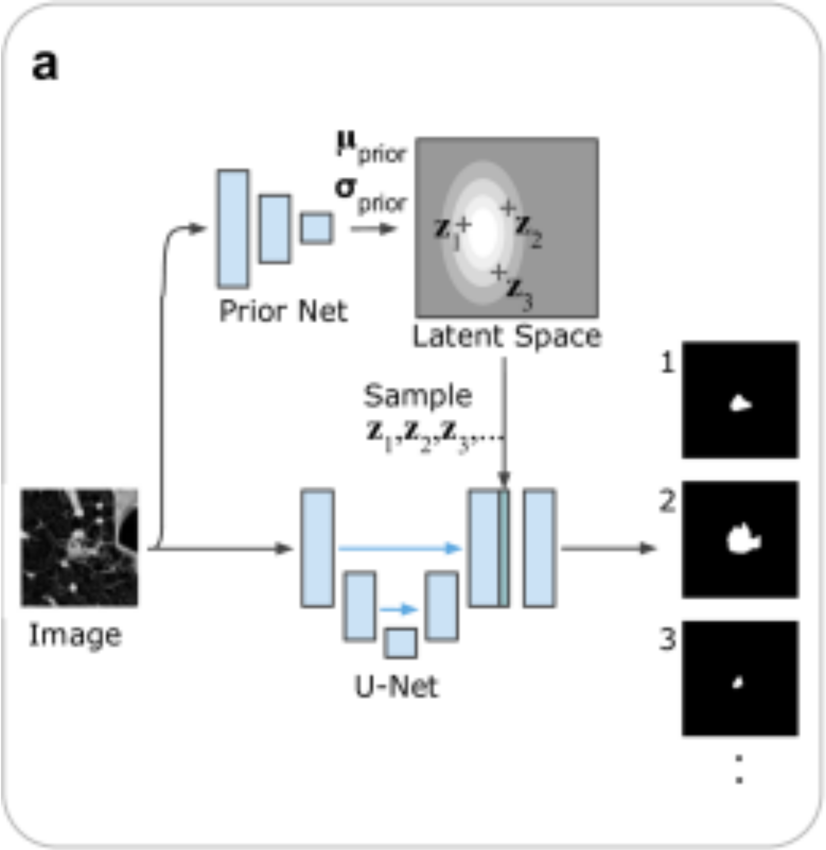
Advancing Science

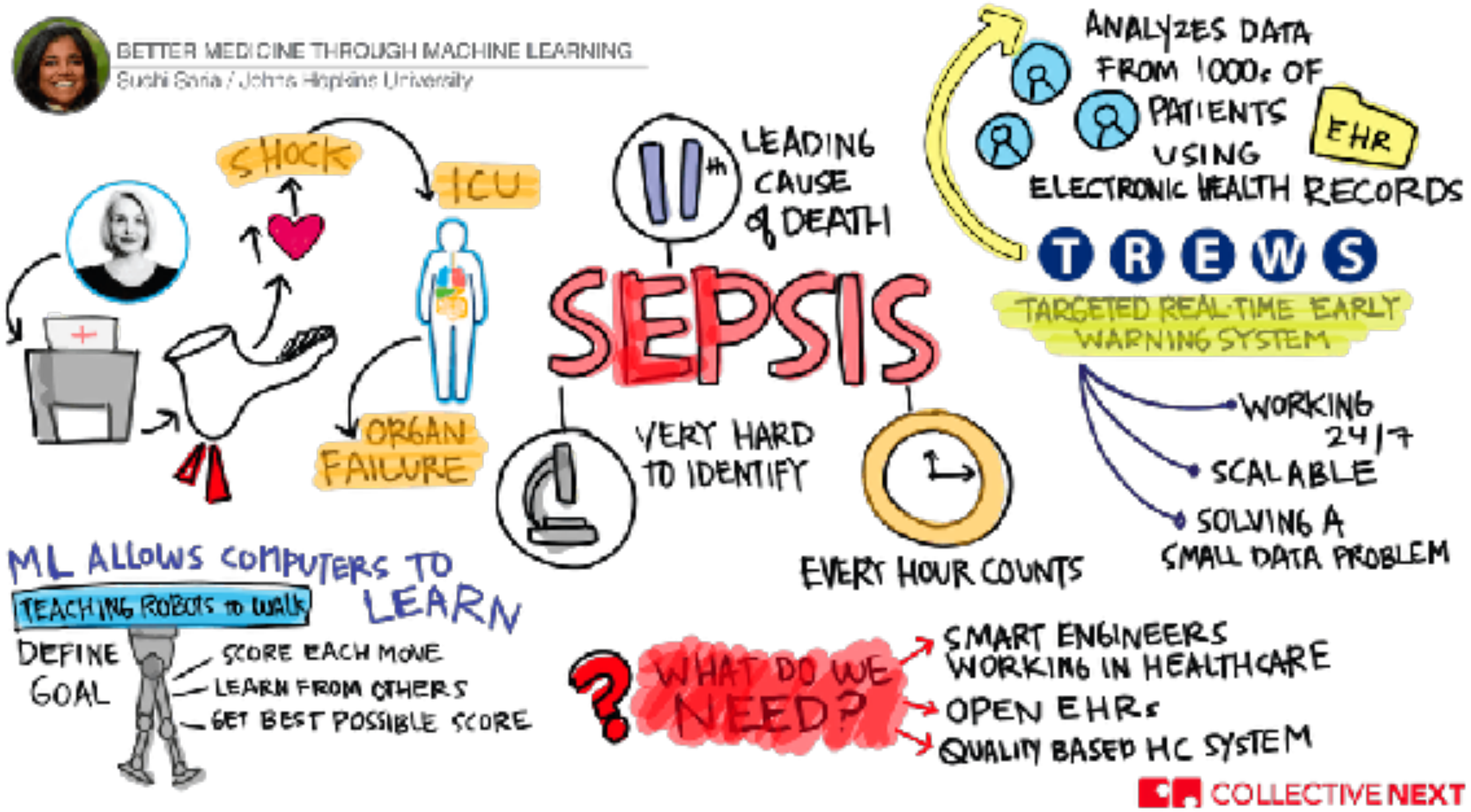






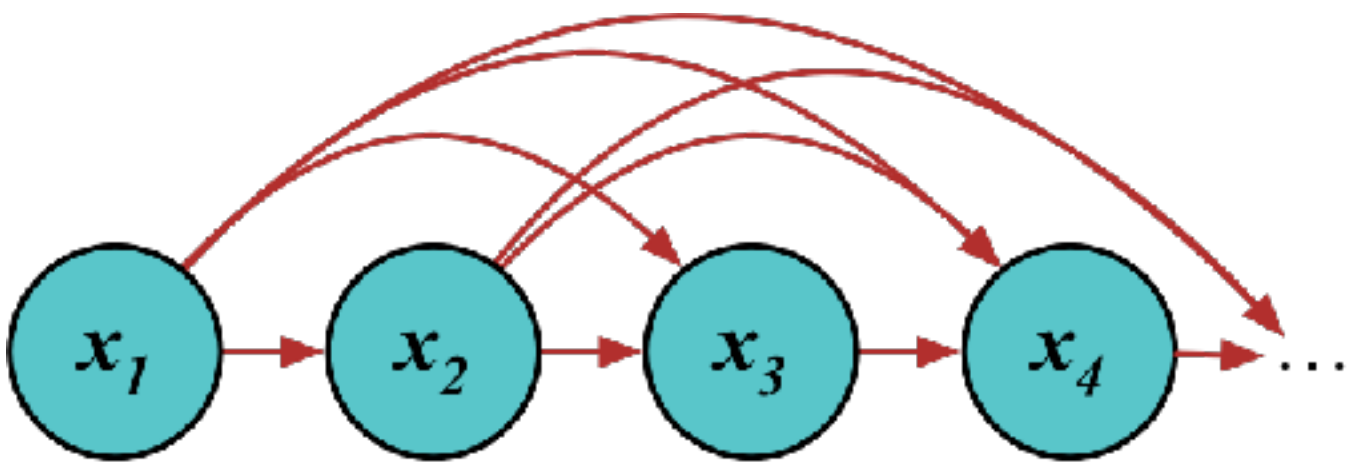
Advancing Healthcare



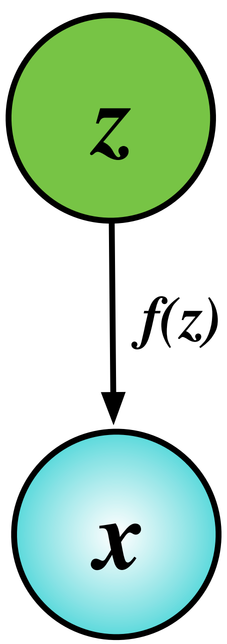


Types of Generative Models

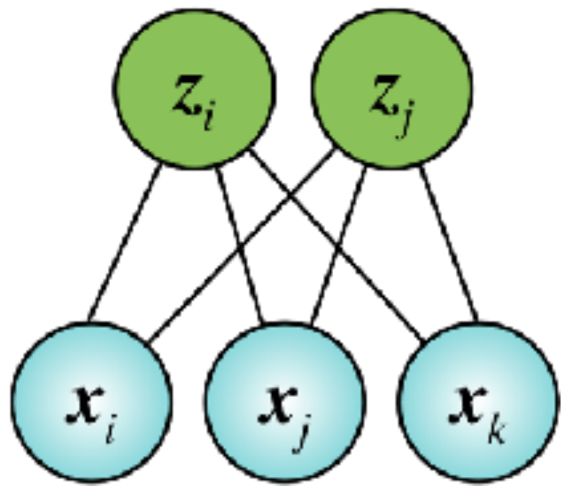
Fully-observed models



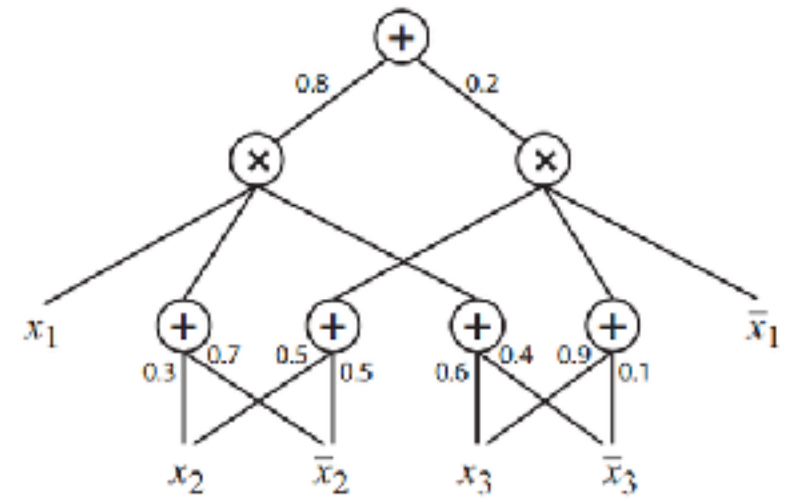
Latent variable models



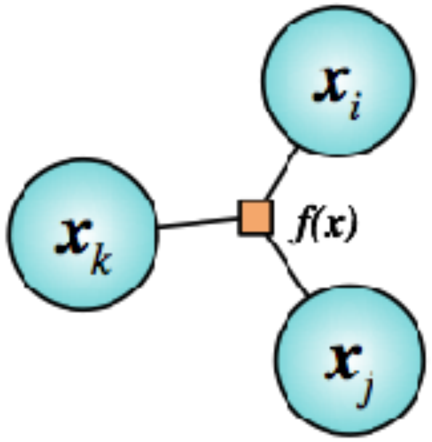
Undirected Models

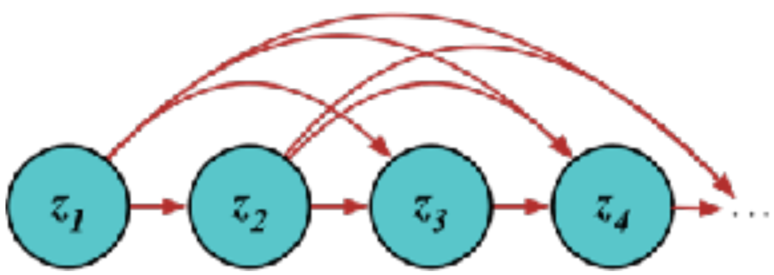


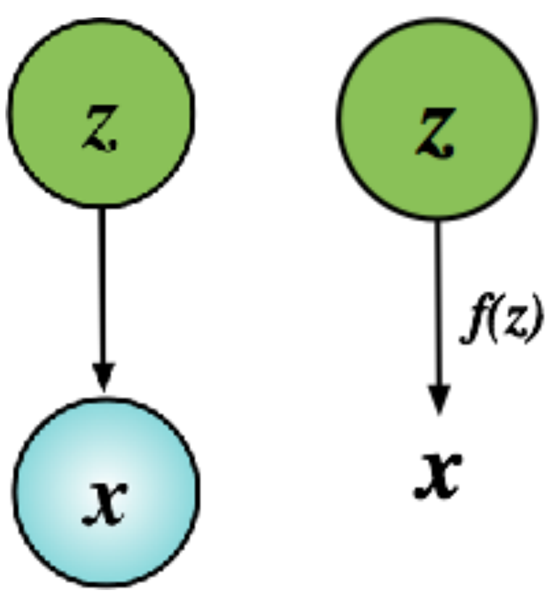
Sum-Product Networks



Types of Generative Models





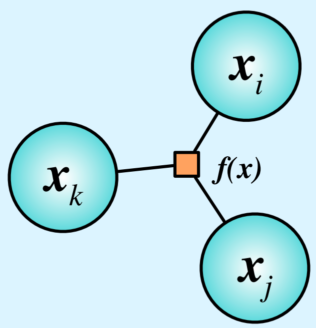


Design Dimensions

- **Data**: binary, real-valued, nominal, strings, images.
- **Dependency**: independent, sequential, temporal, spatial.
- **Representation**: continuous or discrete
- **Dimension**: parametric or non-parametric

- Computational complexity
- Modelling capacity
- Bias, uncertainty, calibration
- Interpretability

Fully-observed Models



Fully-observed models

Model observed data directly **without** introducing any new unobserved **local variables**.

Model Parameters are **global variables.**

Stochastic activations & unobserved random variables are **local variables.**

Markov Models

$$x_1 \sim \mathrm{Cat}(x_1|\pi)$$

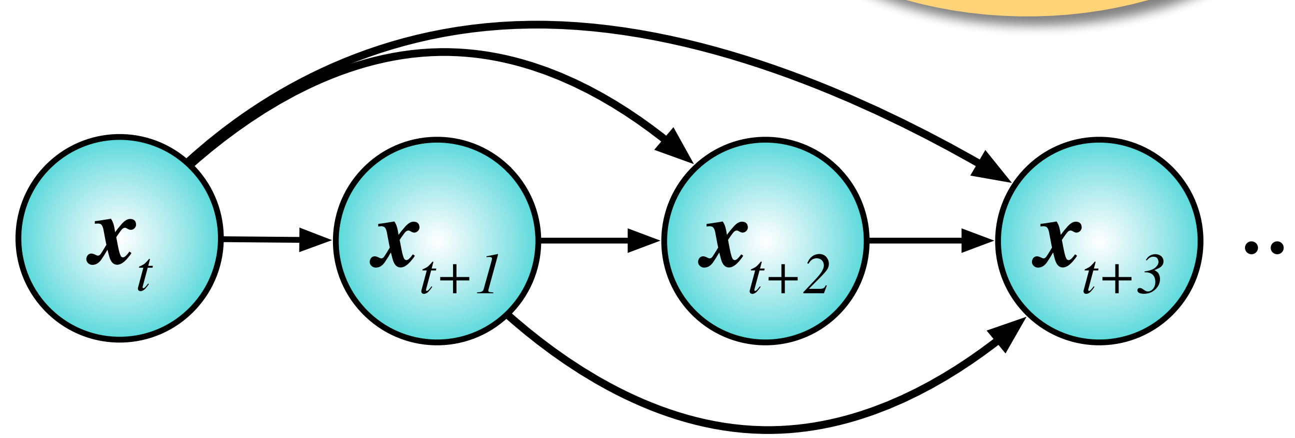
$$x_2 \sim \mathrm{Cat}(x_2|\pi(\mathbf{x}_1))$$

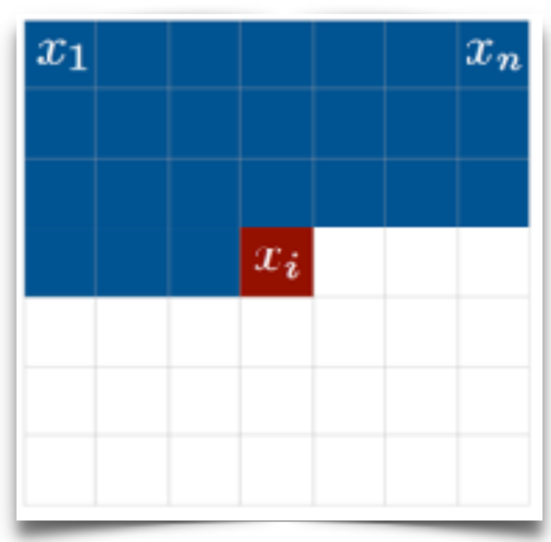
$$\cdots$$

$$x_i \sim \mathrm{Cat}(x_i|\pi(\mathbf{x}_{<n}))$$

$$p(\mathbf{x}) = \prod_i p(x_i|f(\mathbf{x}_{<i};\boldsymbol{\theta}))$$

All conditional probabilities described by deep networks.





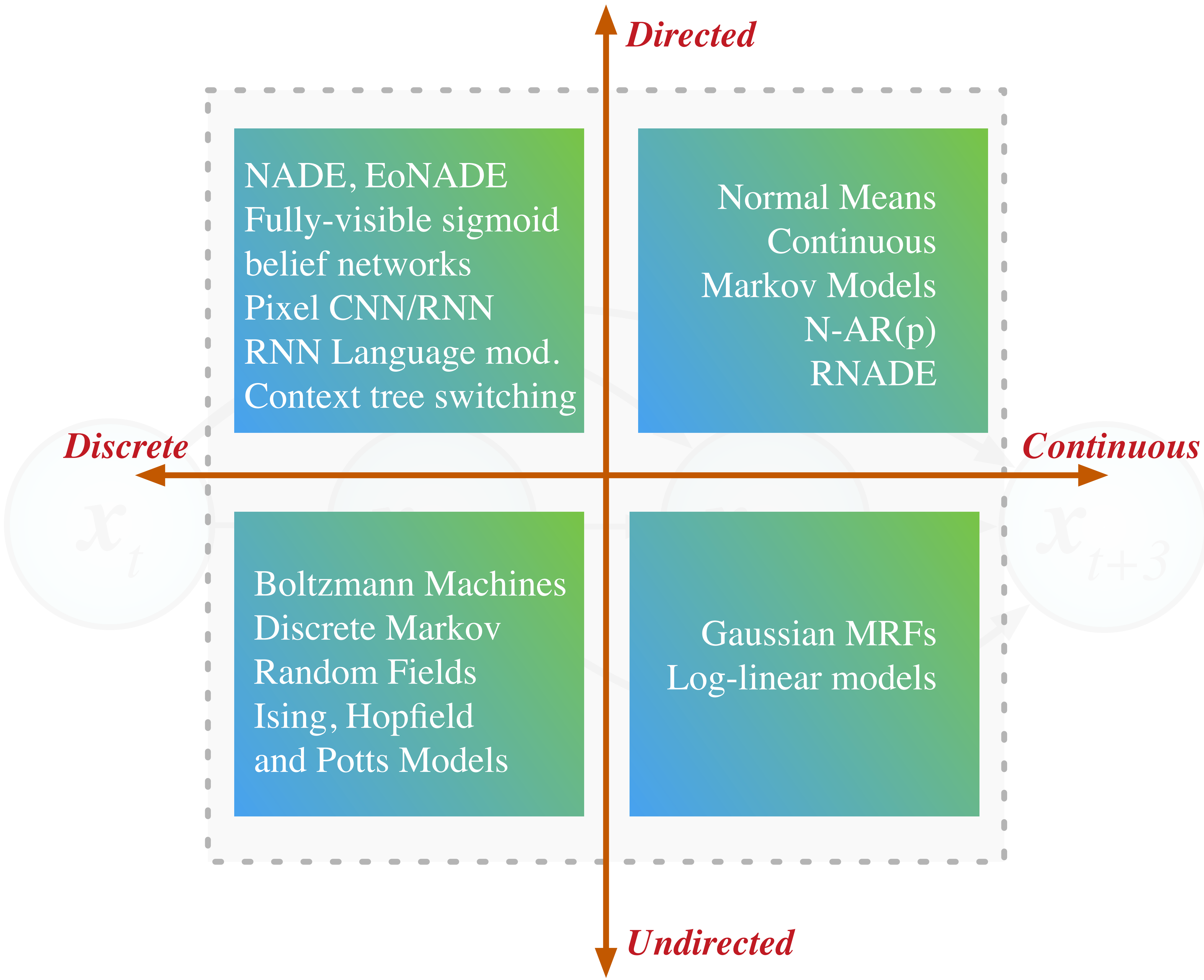
Pixel CNN

Hartebeest

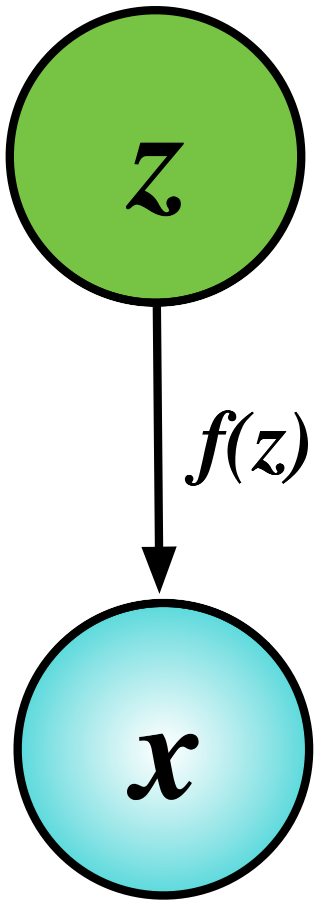
White Whale

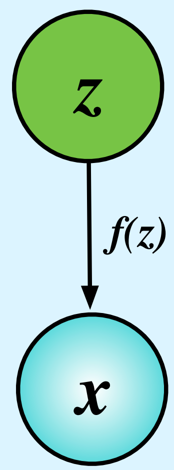
Properties

+ Can directly encode how observed points are related.
+ *Any data* type can be used
+ For directed graphical models:
  + **Parameter learning simple**: Log-likelihood is directly computable, no approximation needed.
  + Easy to scale-up to large models, many optimisation tools available.
  - Order sensitive.
- For undirected models,
  - **Parameter learning difficult**: Need to compute normalising constants.
- **Generation can be slow**: iterate through elements sequentially, or using a Markov chain.


Directed
NADE, EoNADE
Fully-visible sigmoid
belief networks
Pixel CNN/RNN
RNN Language mod.
Context tree switching
Normal Means
Continuous
Markov Models
N-AR(p)
RNADE
Discrete
Continuous
Boltzmann Machines
Discrete Markov
Random Fields
Ising, Hopfield
and Potts Models
Gaussian MRFs
Log-linear models
Undirected

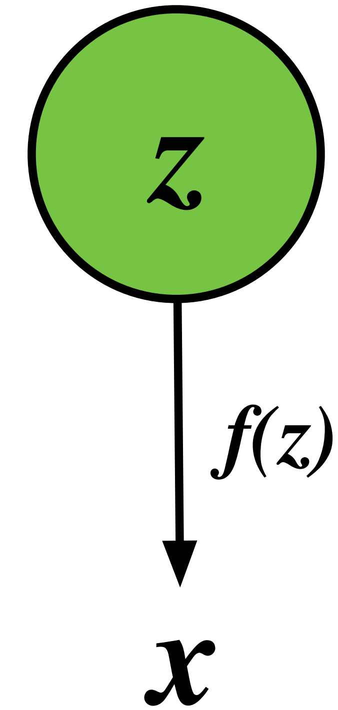
Latent Variable Models





Latent variable models

Introduce an unobserved **local random variables** that represents hidden causes.



Prescribed models

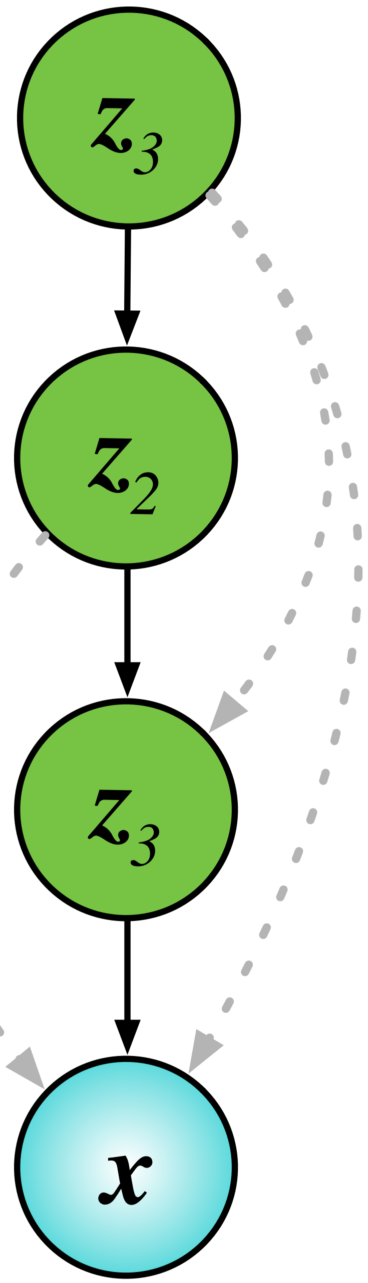
Use observer likelihoods and assume observation noise.

Implicit models

Likelihood-free or simulation-based models.

Prescribed Models

Deep Latent Gaussian Model



$$\mathbf{z}_3 \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$\mathbf{z}_2 | \mathbf{z}_3 \sim \mathcal{N}(\mu(\mathbf{z}_3), \Sigma(\mathbf{z}_3))$$

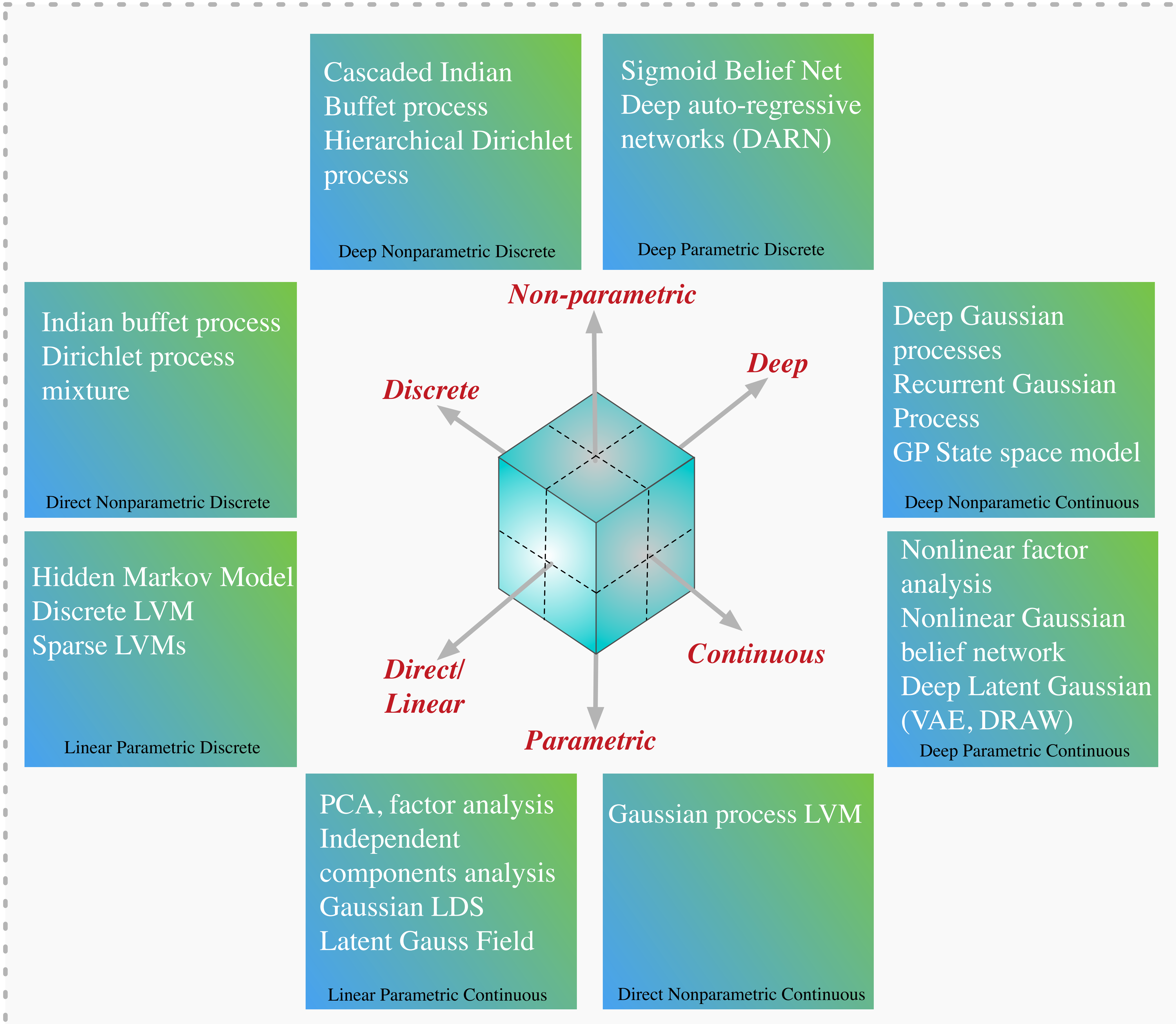
$$\mathbf{z}_1 | \mathbf{z}_2 \sim \mathcal{N}(\mu(\mathbf{z}_2), \Sigma(\mathbf{z}_2))$$

$$\mathbf{x} | \mathbf{z}_1 \sim \mathcal{N}(\mu(\mathbf{z}_1), \Sigma(\mathbf{z}_1))$$

Convolutional DRAW

Properties

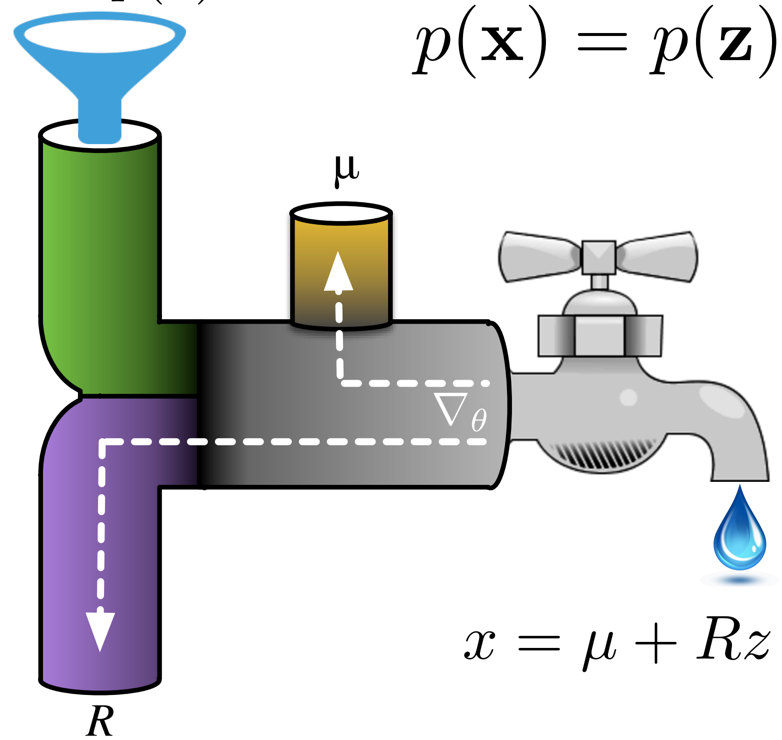
- + Easy sampling.
- + Easy way to include hierarchy and depth.
- + Easy to encode structure believed to generate the data
- + Avoids order dependency assumptions: marginalisation of latent variables induces dependencies.
- + Latents provide compression and representation the data.
- + Scoring, model comparison and selection possible using the marginalised likelihood.
- - Inversion process to determine latents corresponding to a input is difficult in general
- - Difficult to compute marginalised likelihood requiring approximations.
- - Not easy to specify rich approximations for latent posterior distribution.


Cascaded Indian Buffet process
Hierarchical Dirichlet process
Deep Nonparametric Discrete
Sigmoid Belief Net
Deep auto-regressive networks (DARN)
Deep Parametric Discrete
Indian buffet process
Dirichlet process mixture
Direct Nonparametric Discrete
Non-parametric
Discrete
Deep
Direct/ Linear
Continuous
Parametric
Deep Gaussian processes
Recurrent Gaussian Process
GP State space model
Deep Nonparametric Continuous
Hidden Markov Model
Discrete LVM
Sparse LVMs
Linear Parametric Discrete
Nonlinear factor analysis
Nonlinear Gaussian belief network
Deep Latent Gaussian (VAE, DRAW)
Deep Parametric Continuous
PCA, factor analysis
Independent components analysis
Gaussian LDS
Latent Gauss Field
Linear Parametric Continuous
Gaussian process LVM
Direct Nonparametric Continuous

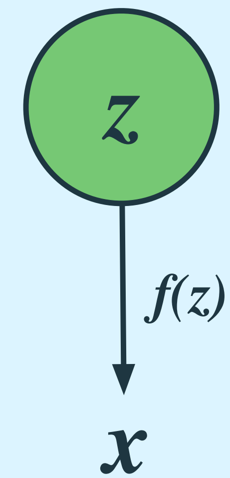
Implicit Models

Change of variables for invertible functions

$$p(\mathbf{x}) = p(\mathbf{z}) \left| \det \frac{\partial f}{\partial \mathbf{z}} \right|^{-1}$$



$$x = \mu + Rz$$



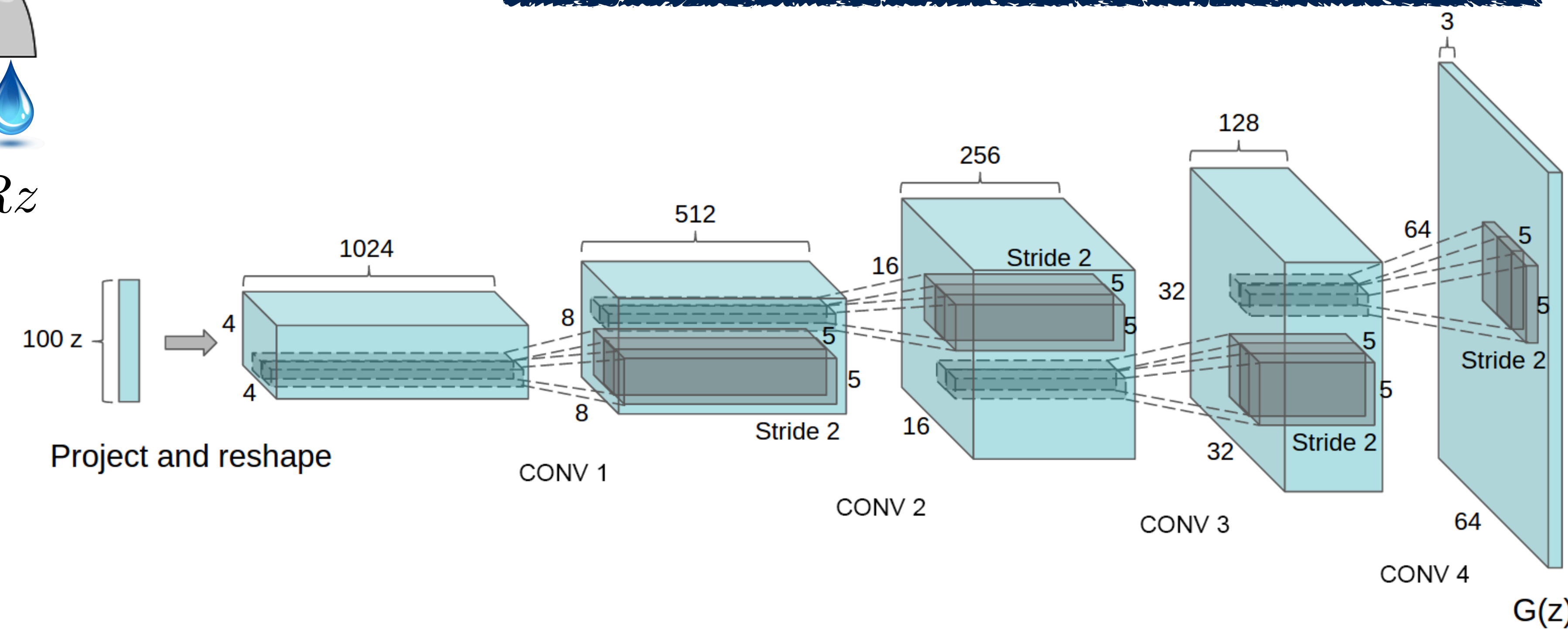
Implicit models

Transform an unobserved **noise source** using a parameterised **function**.

Generator Networks

$$\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$\mathbf{x} = f(\mathbf{z}; \boldsymbol{\theta})$$



The transformation function is parameterised by a linear or deep network (fully-connected, convolutional or recurrent).

Properties

+ Easy sampling, and natural to specify.
+ Easy to compute expectations without knowing final distribution.
+ Can exploit with large-scale classifiers and convolutional networks.
- ***Difficult to satisfy constraints***: Difficult to maintain invertibility, and challenging optimisation.
- ***Lack of noise model*** (likelihood):
  - Difficult to extend to generic data types
  - Difficult to account for noise in observed data.
  - Hard to compute marginalised likelihood for model scoring, comparison and selection.

Convolutional generative adversarial network

Bedrooms

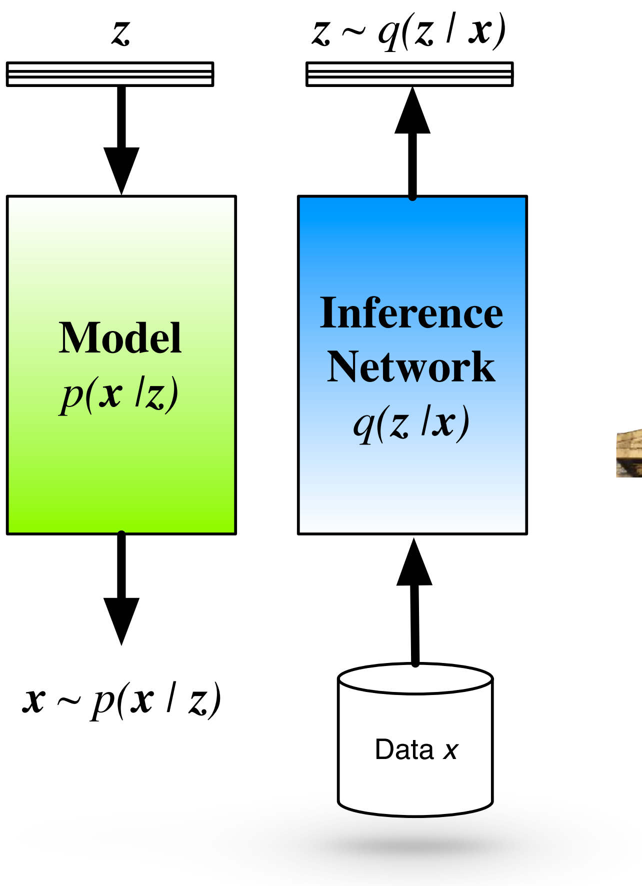
Stochastic
Differential Equations
Hamiltonian and
Langevin SDE
Diffusion Models
Non- and volume
preserving flows

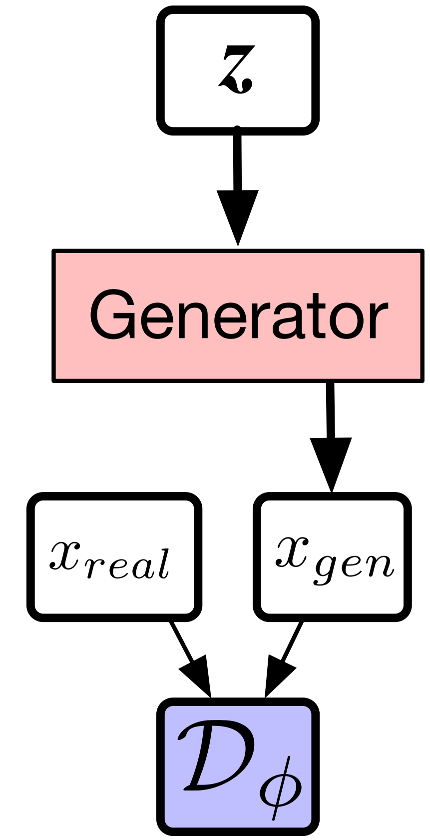
One-liners and
inverse sampling
Distrib. warping
Normalising flows
GAN generator nets
Non- and volume
preserving transforms

Diffusions
Continuous time

Functions
Discrete time

Model-Inference-Algorithm





Prescribed latent variable models + variational inference

Variational Autoencoders (VAEs)

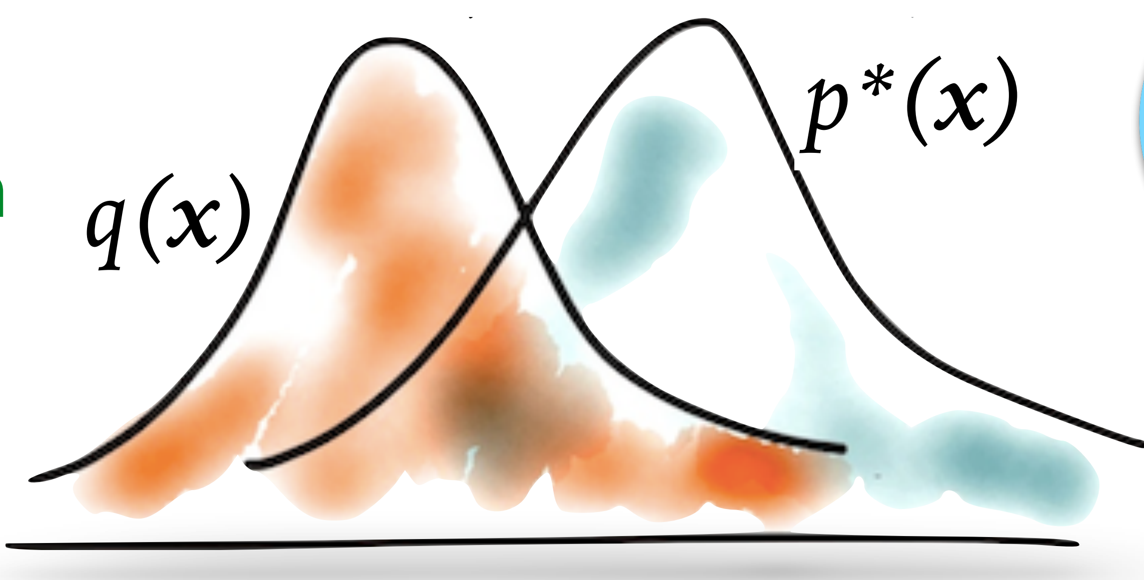
Implicit latent variable models + estimation-by-comparison

Generative Adversarial Networks (GANs)

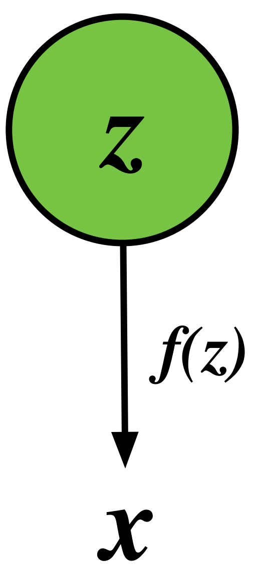
Learning by Comparison

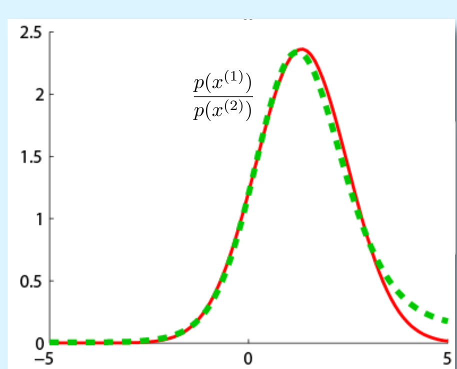
Implicit latent variable models + **estimation-by-comparison**

We compare the estimated distribution q(x) to the true distribution p*(x) using samples.



Basic idea:
Transform into learning a model of the density ratio.





Learning principle: Two-sample tests

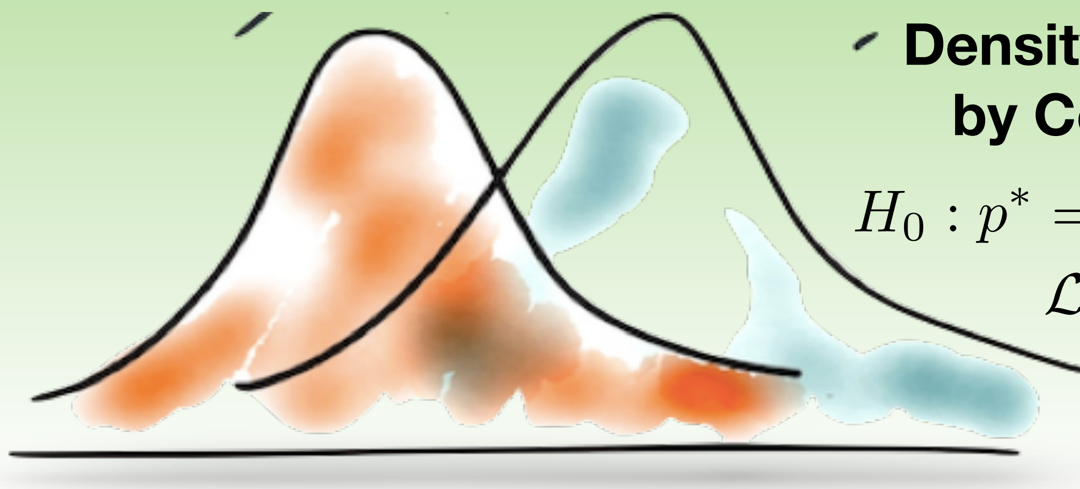
$$\frac{p^*(\mathbf{x})}{q(\mathbf{x})} = 1 \qquad p^*(\mathbf{x}) = q(\mathbf{x})$$

Interest is not in estimating the marginal probabilities, only in how they are related.

Estimation by Comparison

Two steps

1. Use a hypothesis **test or comparison** to obtain some model to tells how data from our model differs from observed data.



Density Estimation by Comparison

$$H_0 : p^* = q_\theta \text{ vs. } p^* \neq q_\theta$$

$$\mathcal{L}(\theta, \phi)$$

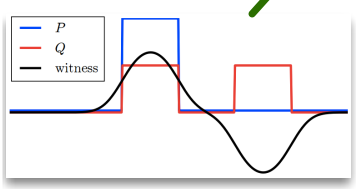
Density Difference

$$r_\phi = p^* - q_\theta$$

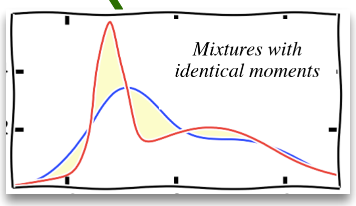
Density Ratio

$$r_\phi = \frac{p^*}{q_\theta}$$

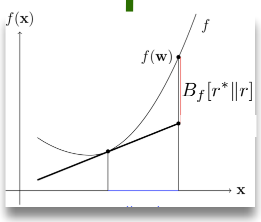
2. **Adjust model** to better match the data distribution using the comparison model from step 1.



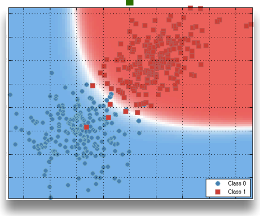
Max Mean Discrepency



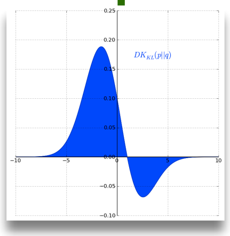
Moment Matching



Bregman Divergence



Class Probability Estimation



f-Divergence

$$f(u) = u \log u - (u+1)\log(u+1)$$

Adversarial Learning

$$\frac{p^*(\mathbf{x})}{q(\mathbf{x})} = \frac{p(y=1|\mathbf{x})}{p(y=-1|\mathbf{x})}$$

$$p(y=+1|\mathbf{x}) = D_\theta(\mathbf{x}) \quad p(y=-1|\mathbf{x}) = 1 - D_\theta(\mathbf{x})$$

Scoring Function

$$\mathcal{F}(\mathbf{x}, \theta, \phi) = \mathbb{E}_{p^*(x)}[\log D_\theta(\mathbf{x})] + \mathbb{E}_{q_\phi(x)}[\log(1 - D_\theta(\mathbf{x})]$$

Bernoulli Loss

Generative Adversarial Networks

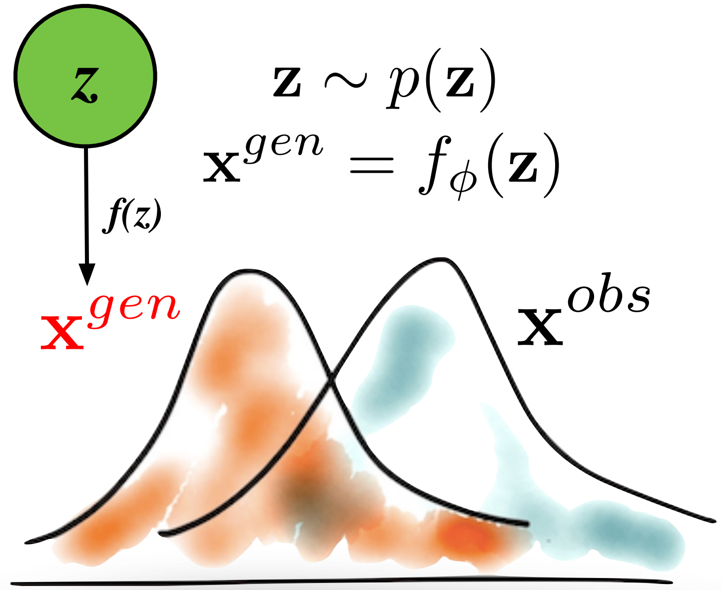
Alternating optimisation $\min_\phi \max_\theta \mathcal{F}(\mathbf{x}, \theta, \phi)$

Comparison loss $\theta \propto \nabla_\theta \mathbb{E}_{p^*(x)}[\log D_\theta(\mathbf{x})] + \nabla_\theta \mathbb{E}_{q_\phi(x)}[\log(1 - D_\theta(\mathbf{x})]$

Generative loss $\phi \propto -\nabla_\phi \mathbb{E}_{q(z)}[\log(1 - D_\theta(f_\phi(\mathbf{z}))]$

Instances of testing and inference:

- Unsupervised-as-supervised learning
- Classifier ABC
- Noise-contrastive estimation
- Adversarial learning and GANs



Density-ratio

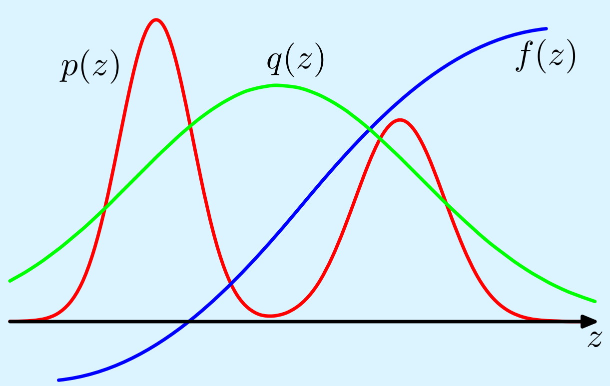
Reparameterisation

Model Evidence

Prescribed latent variable models + variational inference

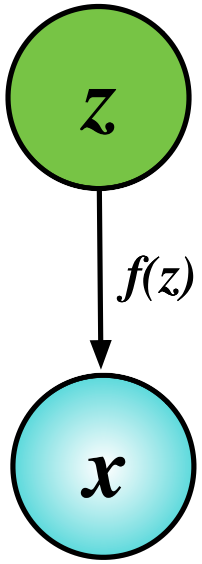
Model evidence (or marginal likelihood, partition function): Integrating out any global and local variables enables model scoring, comparison, selection, moment estimation, normalisation, posterior computation and prediction.

Improve the model evidence for given data samples.



Learning principle: Model Evidence

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$



Integral is intractable in general and requires approximation.

Basic idea:
Transform the integral into an expectation over a simple, known distribution.

Variational Inference

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

$$\boxed{\mathcal{F}(\mathbf{x}, q) = \mathbb{E}_{q(\mathbf{z})}[\log p(\mathbf{x}|\mathbf{z})] - KL[q(\mathbf{z}) \| p(\mathbf{z})]}$$

This bound is exactly of the form we are looking for.

- **Variational free energy:** We obtain a functional and are free to choose the distribution *q(z)* that best matches the true posterior.
- **Evidence lower bound (ELBO):** principled bound on the marginal likelihood, or model evidence.
- Certain choices of q(z) makes this quantity easier to compute. Examples to come.

Identity Bounding

Variational Bound

Interpreting the bound:

$$\mathcal{F}(\mathbf{x}, q) = \boxed{\mathbb{E}_{q(\mathbf{z})}[\log p(\mathbf{x}|\mathbf{z})]} - \boxed{KL[q(\mathbf{z})\|p(\mathbf{z})]}$$

Approx. Posterior

Reconstruction

Penalty

- **Approximate posterior distribution *q(z)*:** Best match to true posterior *p(z|y)*, one of the unknown inferential quantities of interest to us.
- **Reconstruction cost**: The expected log-likelihood measure how well samples from *q(z)* are able to explain the data *y*.
- **Penalty:** Ensures the the explanation of the data *q(z)* doesn't deviate too far from your beliefs *p(z)*. A mechanism for realising Okham's razor.

Variational Bound

$$\mathcal{F}(\mathbf{x}, q) = \underbrace{\mathbb{E}_{q(\mathbf{z})}[\log p(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction}} - \underbrace{KL[q(\mathbf{z})\|p(\mathbf{z})]}_{\text{Penalty}}$$

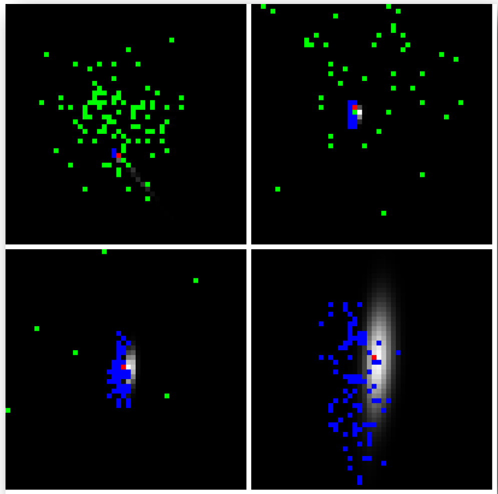
Approx. Posterior

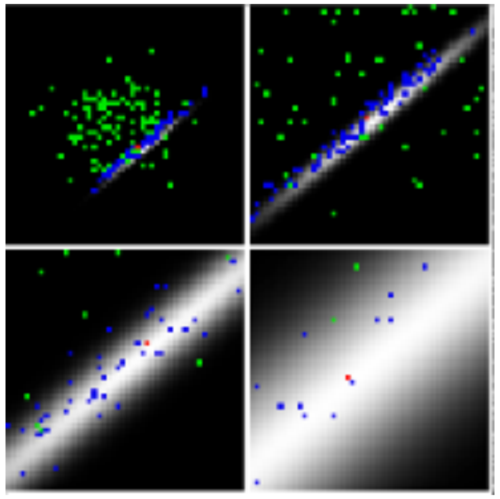
Some comments on *q*:

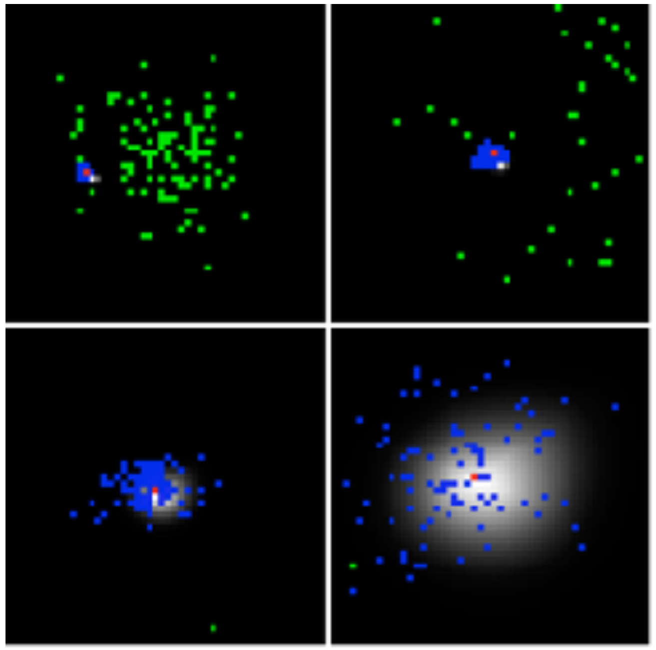
- **Integration is now optimisation**: optimise for *q(z)* directly.
  - I write *q(z)* to simplify the notation, but it depends on the data, *q(z|x)*.
  - *Easy convergence assessment* since we wait until the free energy (loss) reaches convergence.
- **Variational parameters:** parameters of *q(z)*
  - E.g., if a Gaussian, variational parameters are mean and variance.
  - Optimisation allows us to *tighten the bound* and get as close as possible to the true marginal likelihood.

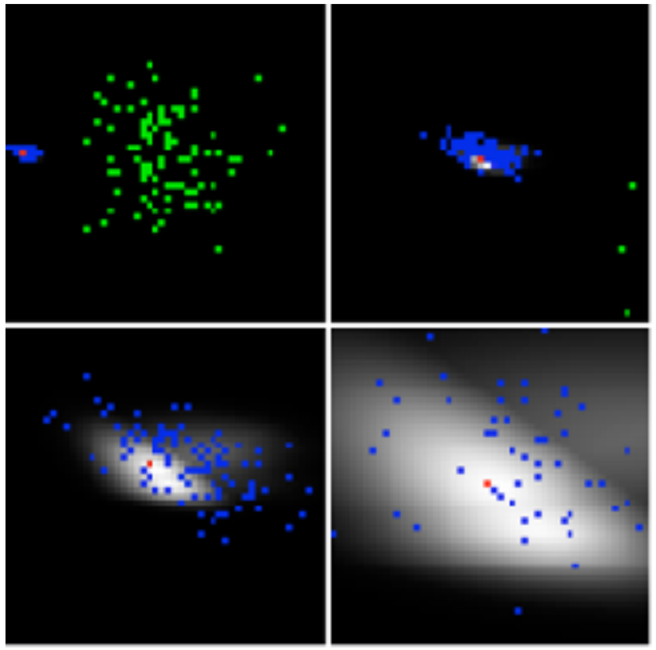
Real Posteriors

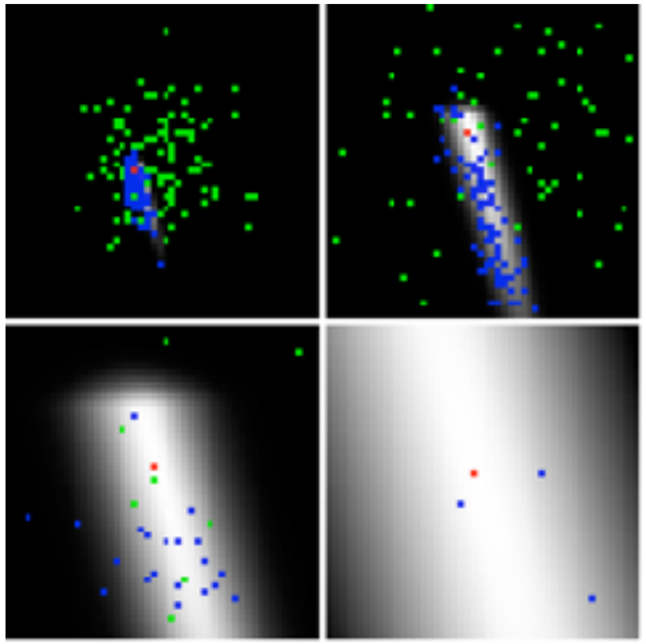
Require flexible approximations for the types of posteriors we are likely to see.







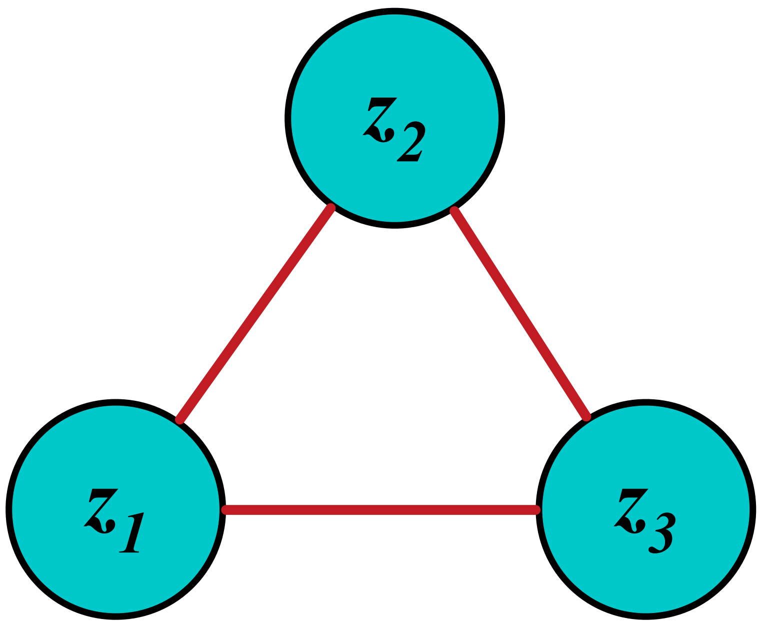


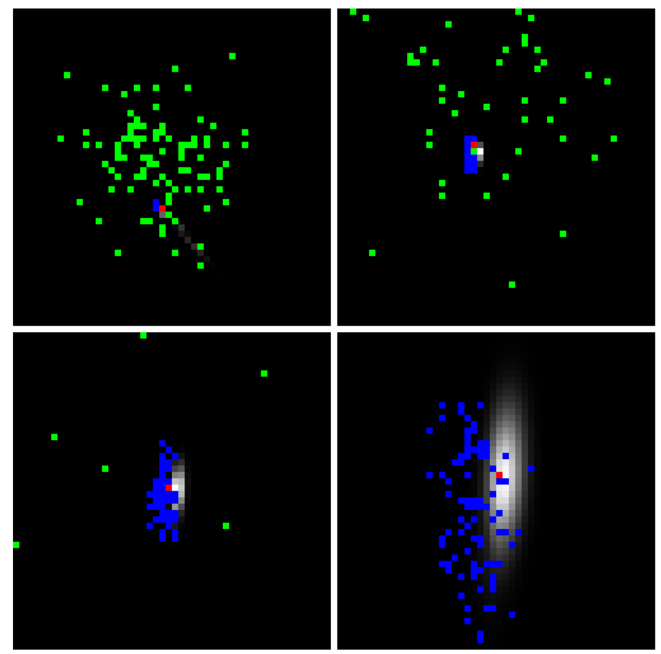


Mean-Fields

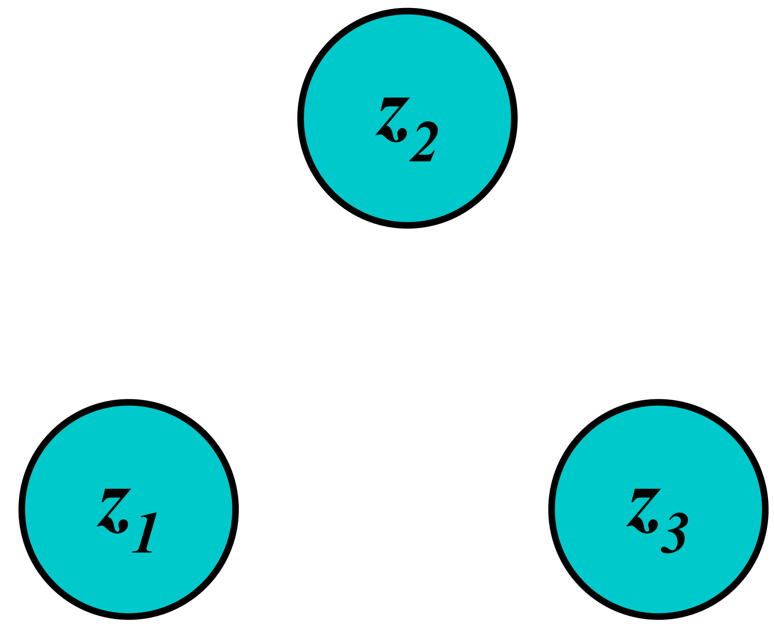
Mean-field methods assume that the distribution is factorised.

True Posterior





Fully-factorised



Most Expressive ⟵⟶ *Least Expressive*

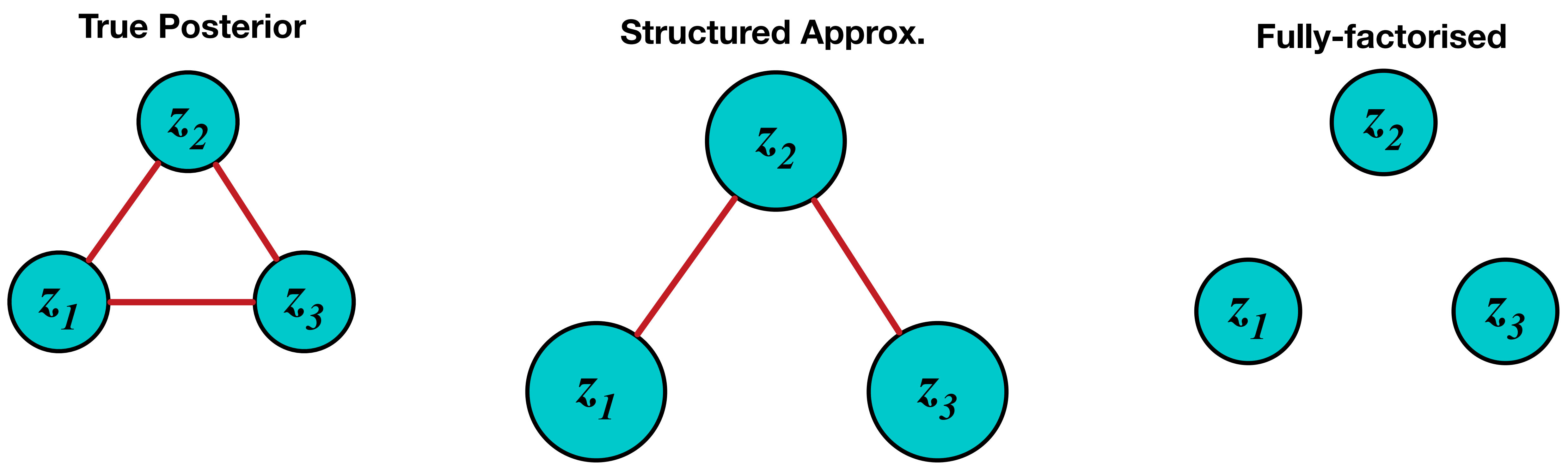
$$q^*(z|x) \propto p(x|z)p(z)$$

$$q_{MF}(z|x) = \prod_k q(z_k)$$

Restricted class of approximations: every dimension (or subset of dimensions) of the posterior is independent.

Structured Mean-field

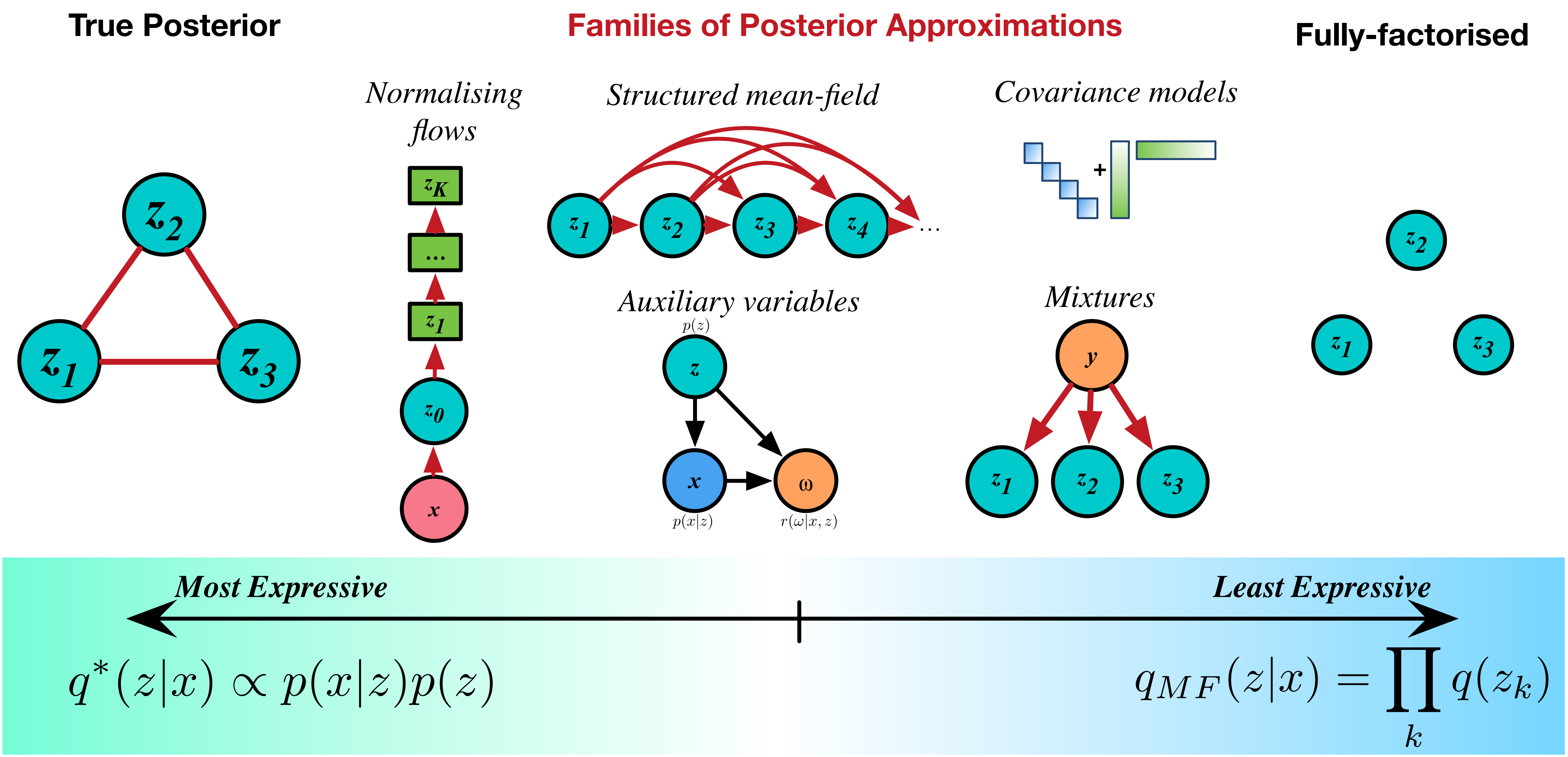
Structured mean-field: introduce dependencies into our factorisation.



Most Expressive ⟵ ⟶ *Least Expressive*

$$q^*(z|x) \propto p(x|z)p(z) \qquad q(z) = \prod_k q_k(z_k|\{z_j\}_{j\neq k}) \qquad q_{MF}(z|x) = \prod_k q(z_k)$$

Families of Approximations

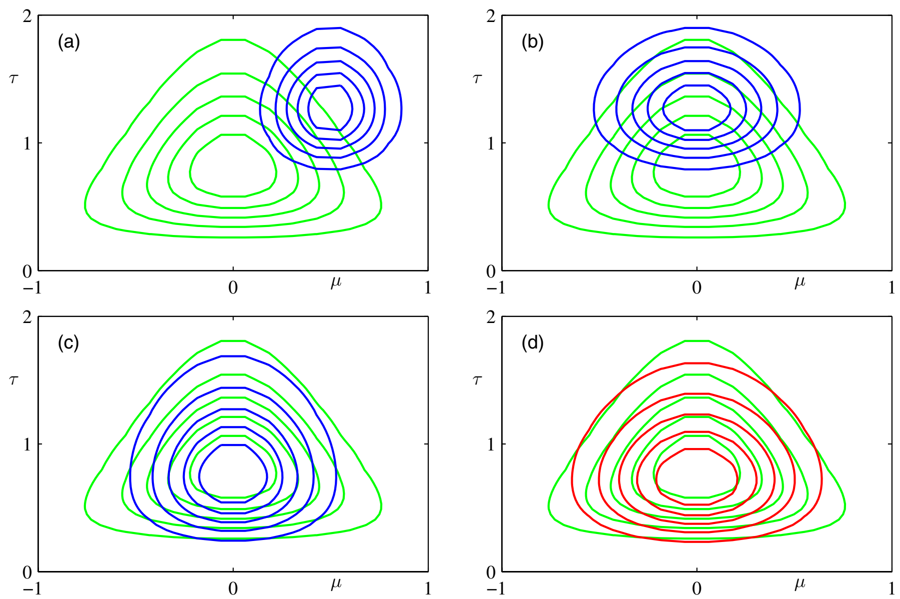


Variational Optimisation

$$\mathcal{F}(\mathbf{x}, q) = \underbrace{\mathbb{E}_{q(\mathbf{z})}[\log p(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction}} - \underbrace{KL[q(\mathbf{z})\|p(\mathbf{z})]}_{\text{Penalty}}$$

Approx. Posterior

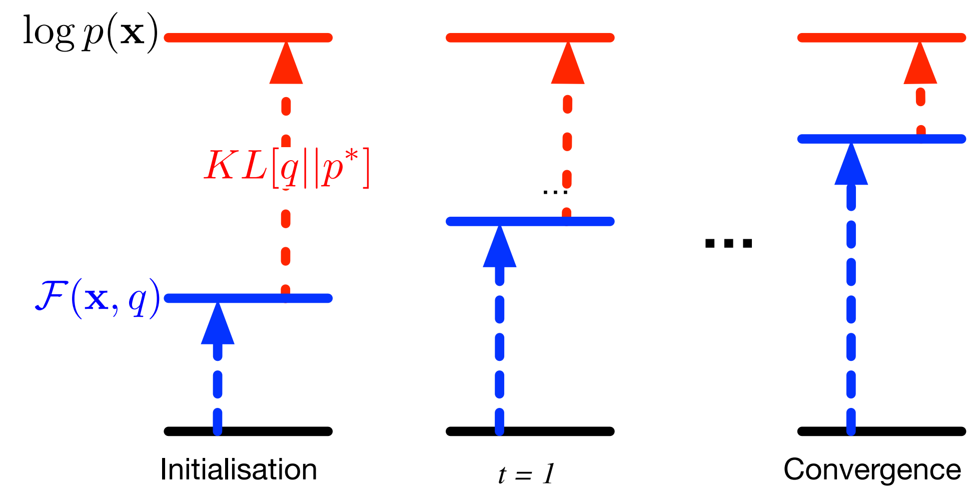
- Variational EM
- Stochastic Variational Inference
- Doubly Stochastic Variational Inference
- Amortised Inference



Variational EM

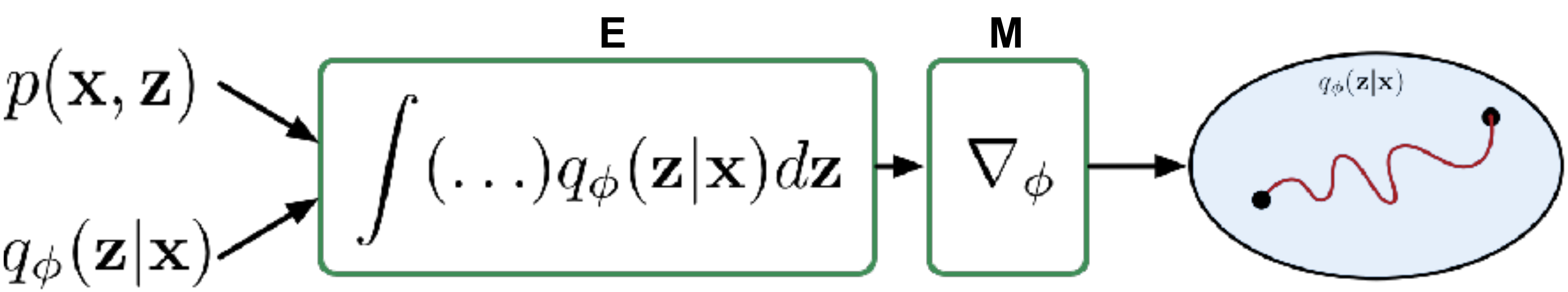
$$\mathcal{F}(\mathbf{x}, q) = \mathbb{E}_{q(\mathbf{z})}[\log p(\mathbf{x}|\mathbf{z})] - KL[q(\mathbf{z})\|p(\mathbf{z})]$$

Alternating optimisation for the variational parameters and then model parameters (VEM).



Repeat:

E-step	$\phi \propto \nabla_\phi \mathcal{F}(\mathbf{x}, q)$	*Var. params*
M-step	$\theta \propto \nabla_\theta \mathcal{F}(\mathbf{x}, q)$	*Model params*



Amortised Inference

Repeat:

E-step (compute q)

For $i = 1, \ldots N$

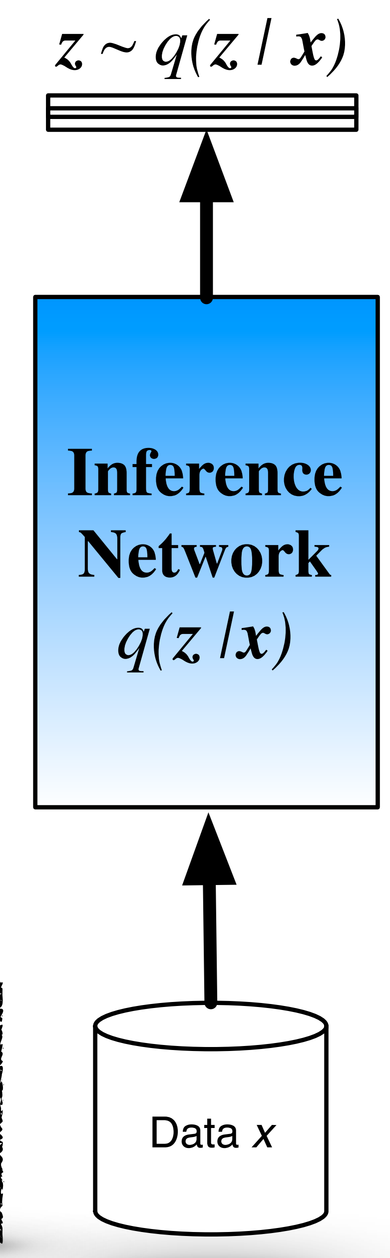
$$\phi_n \propto \nabla_\phi \mathbb{E}_{q_\phi(z)}[\log p_\theta(\mathbf{x}_n|z_n)] - \nabla_\phi KL[q(z_n)\|p(z)]$$

Instead of solving for every observation, amortise using a model.

M-step

$$\theta \propto \frac{1}{N}\sum_n \mathbb{E}_{q_\phi(z)}[\nabla_\theta \log p_\theta(\mathbf{x}_n|z_n)]$$

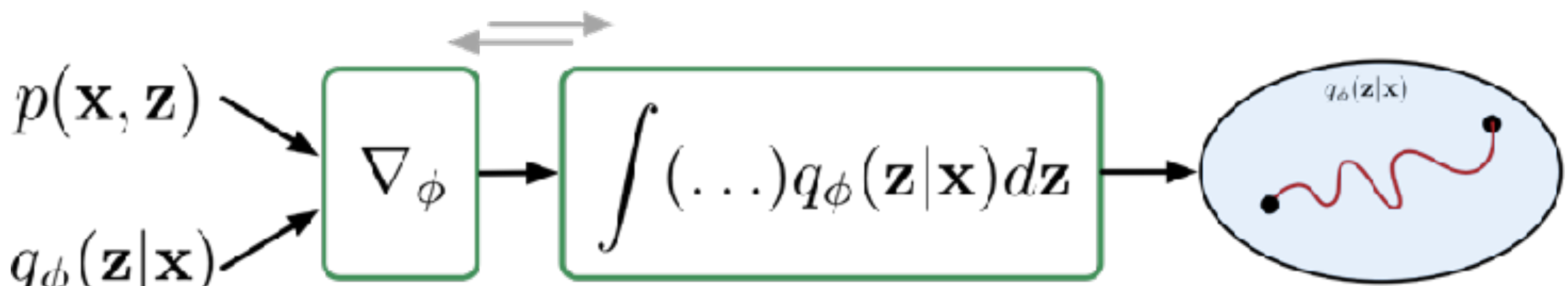
- **Inference network**: *q* is an ***encoder,*** an ***inverse*** model, ***recognition model***.
- Parameters of *q* are now a set of *global parameters* used for inference of all data points - test and train.
- **Amortise (spread) the cost of inference over all data.**
- Joint optimisation of variational and model parameters.



Inference networks provide an efficient mechanism for **posterior inference with memory**

Stochastic Gradients

$$\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z})}[f_\theta(\mathbf{z})] = \nabla \int \boxed{q_\phi(\mathbf{z})}\boxed{f_\theta(\mathbf{z})} d\mathbf{z}$$



Doubly stochastic estimators

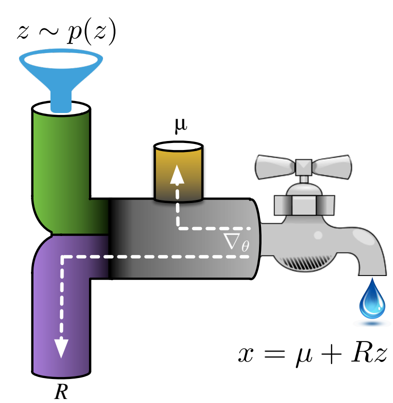
Pathwise Estimator

When easy to use transformation is available and differentiable function *f*.

$$= \mathbb{E}_{p(\epsilon)}[\nabla_\phi f_\theta(g(\epsilon, \phi))]$$

$$z \sim q_\phi(\mathbf{z})$$

$$\mathbf{z} = g(\epsilon, \phi) \quad \epsilon \sim p(\epsilon)$$



Reparameterisation

Score-function estimator

When function *f* non-differentiable and *q(z)* is easy to sample from.

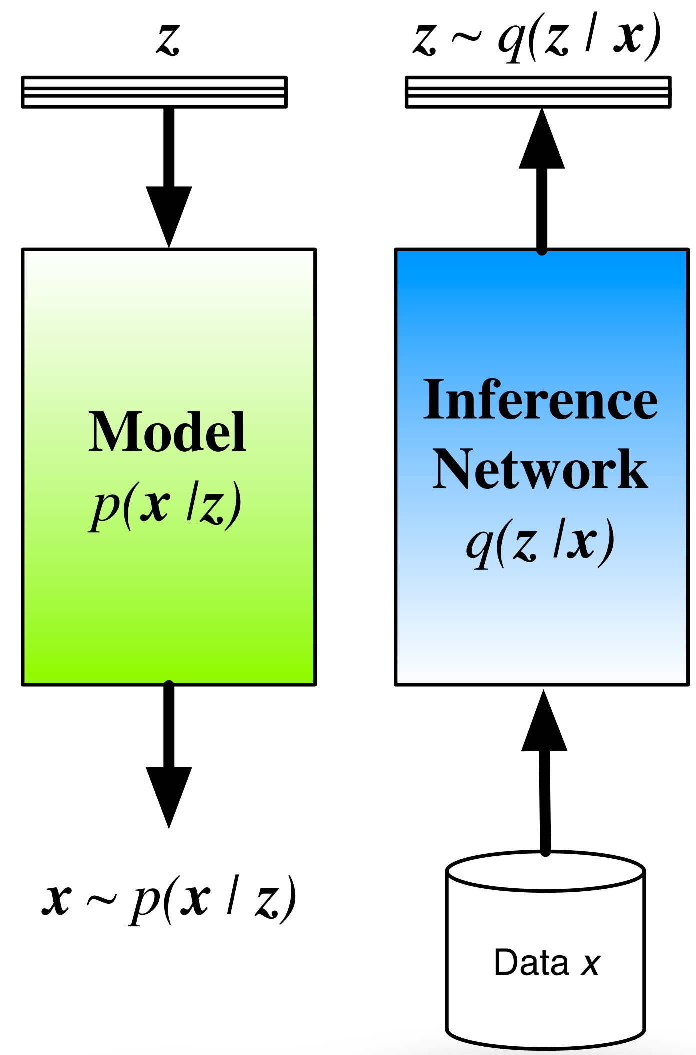
$$= \mathbb{E}_{q(z)}[f_\theta(\mathbf{z}) \nabla_\phi \log q_\phi(\mathbf{z})]$$

Identity **Log-derivative**

Variational Autoencoder

$$\mathcal{F}(\mathbf{x}, q) = \underbrace{\mathbb{E}_{q(\mathbf{z})}[\log p(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction}} - \underbrace{KL[q(\mathbf{z})\|p(\mathbf{z})]}_{\text{Penalty}}$$

Approx. Posterior



Stochastic encoder-decoder system to implement variational inference.

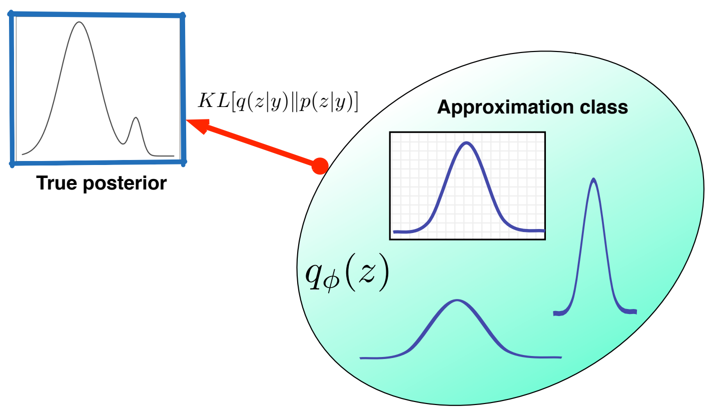
- **Model (Decoder):** likelihood p(**x**|**z**).
- **Inference (Encoder):** variational distribution q(**z**|**x**)
- Transforms an auto-encoder into a generative model

Specific combination of **variational inference** in **latent variable models** using **inference networks**

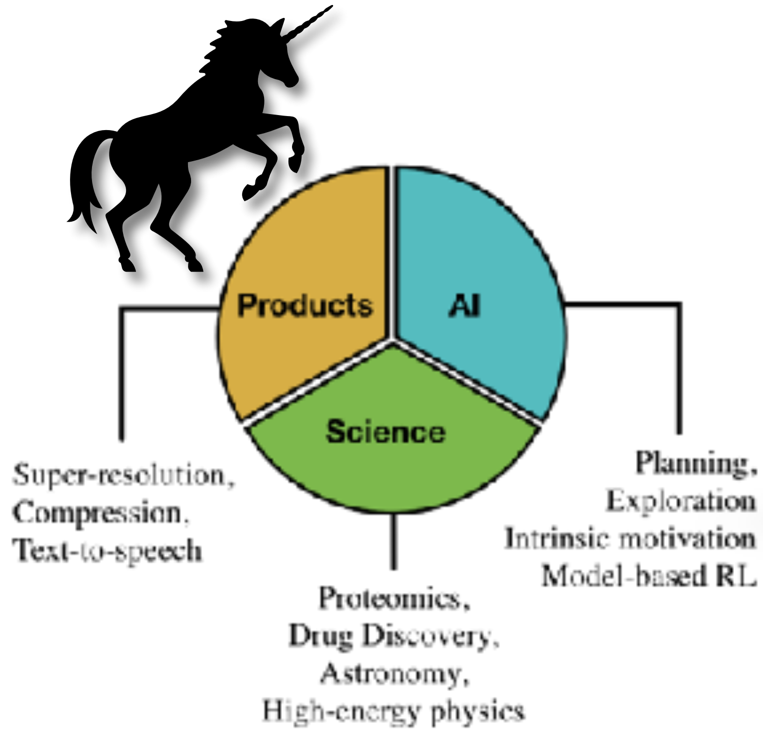
Variational Auto-encoder

But don't forget what your model is, and what inference you use.

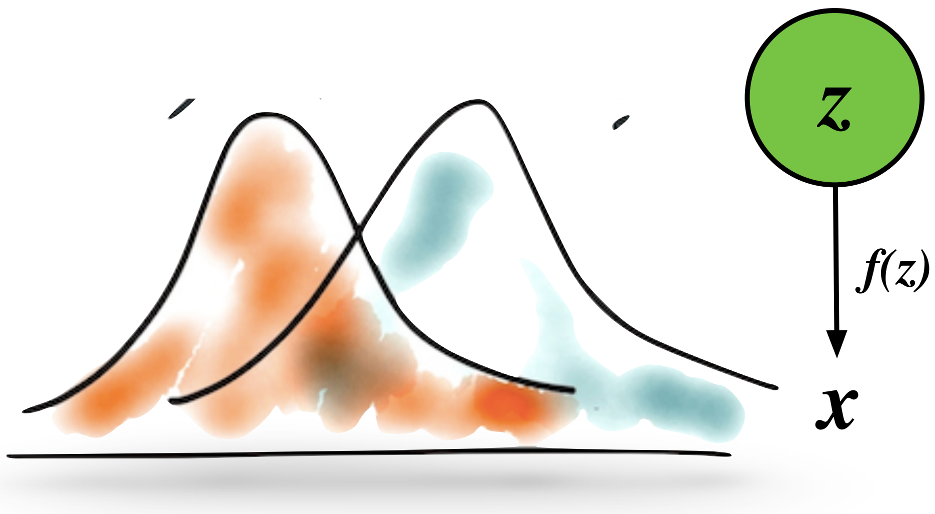
Final Words



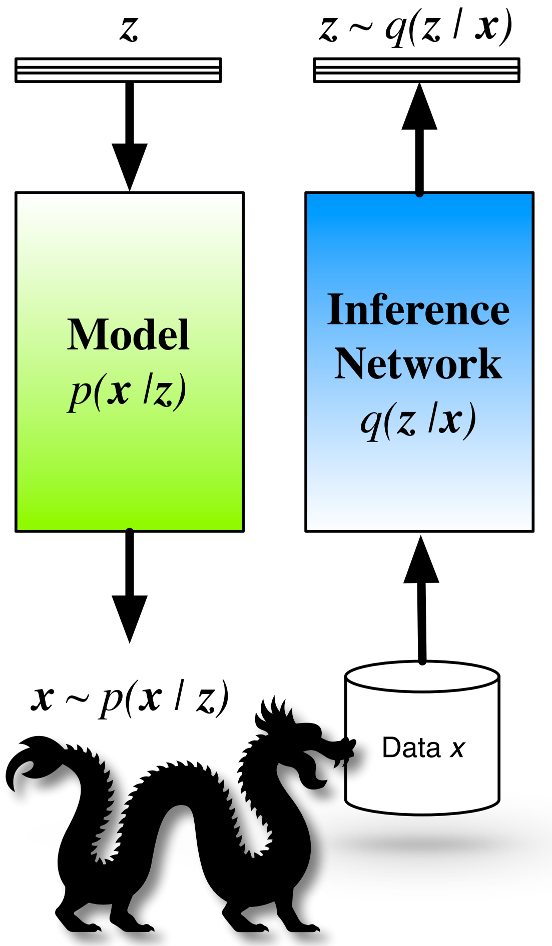
True posterior
$KL[q(z|y)||p(z|y)]$
Approximation class
$q_\phi(z)$



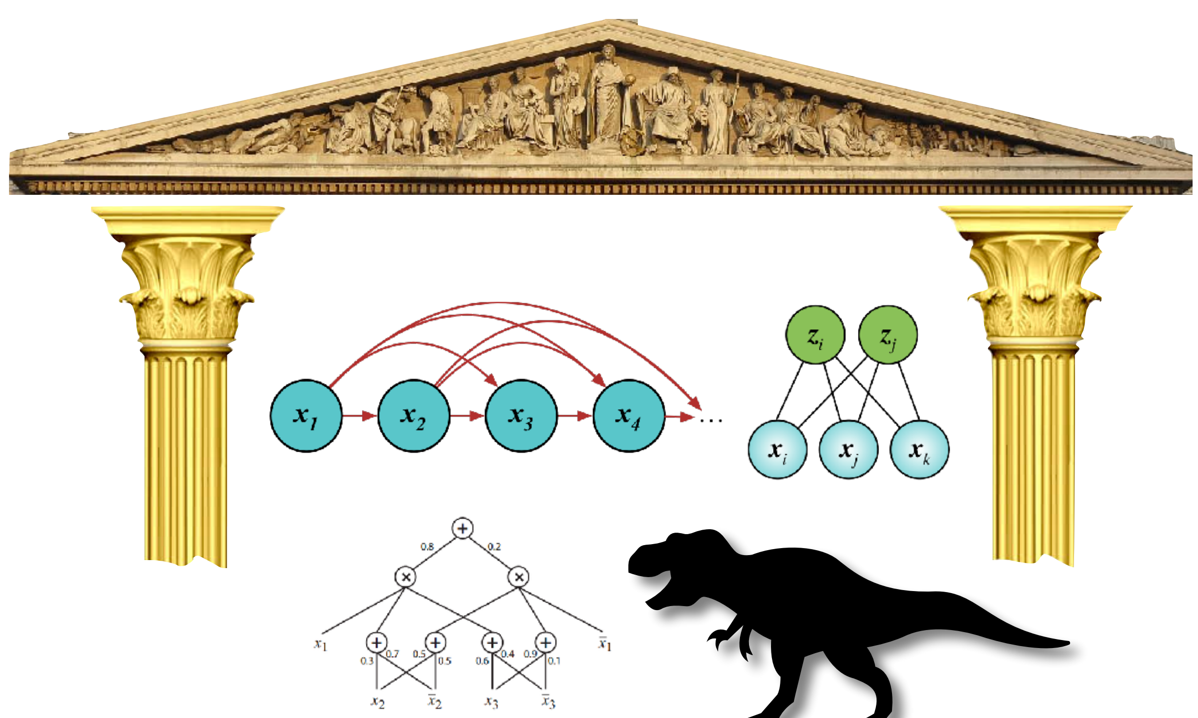
Products
AI
Science
Super-resolution,
Compression,
Text-to-speech
Planning,
Exploration
Intrinsic motivation
Model-based RL
Proteomics,
Drug Discovery,
Astronomy,
High-energy physics

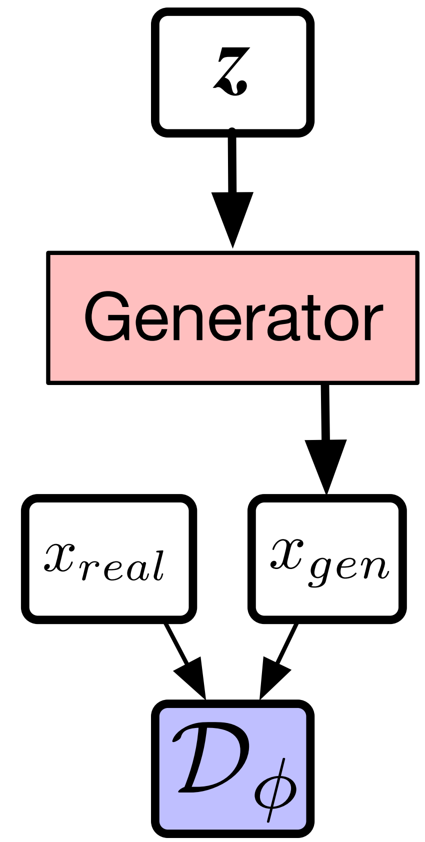


z
f(z)
x



z
z ~ q(z / x)
Model
p(x /z)
Inference
Network
q(z /x)
x ~ p(x / z)
Data x





z
Generator
x_{real}
x_{gen}
$\mathcal{D}_\phi$

shakirm.com/feedback

Generative Models

Foundations | Tricks | Algorithms

Shakir Mohamed

Research Scientist, DeepMind

@shakir_za

DeepMind

Not exhaustive list, and many references to be updated.

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